PALM INTRANET

Day : Thursday
Date: 6/1/2006
Time: 11:41:30

Inventor Information for 10/724971

Inventor Name	City	State/Country
COURNOYER, RICHARD LEO	SAN FRANCISCO	CALIFORNIA
LOUGHHEAD, DAVID GARRETT	BELMONT	CALIFORNIA
O'YANG, COUNDE	SUNNYVALE	CALIFORNIA

Appln Info | Contents | Petition Info | Atty/Agent Info | Continuity Data | Foreign Data

Search Another: Application# Search **or Patent#** Search

PCT / / Search **or PG PUBS #** Search

Attorney Docket # Search

Bar Code # Search

6/1/06

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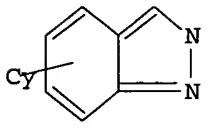

Structure attributes must be viewed using STN Express query preparation.

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L1                STRUCTURE UPLOADED
L2             17 S L1
L3            322 S L1 FUL
L4            265 S L3 AND CAPLUS/LC
L5             57 S L3 NOT L4
L6              0 S L5 AND CAOLD/LC

     FILE 'CAPLUS' ENTERED AT 10:54:38 ON 01 JUN 2006
L7             30 S L3
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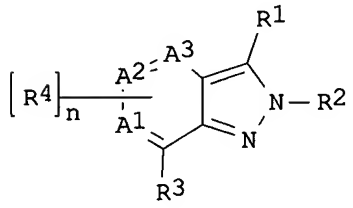
6/1/06

L7 ANSWER 10 OF 30 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:158645 CAPLUS
DOCUMENT NUMBER: 142:261532
TITLE: Preparation of benzoindazole compounds as gabanergic modulators
INVENTOR(S): Lin, Xiao-fa; Loughhead, David Garrett; Novakovic, Sanja; O'Yang, Counde; Putman, David George; Soth, Michael
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005016892	A1	20050224	WO 2004-EP8767		20040805
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004265101	A1	20050224	AU 2004-265101		20040805
CA 2535406	AA	20050224	CA 2004-2535406		20040805
EP 1656353	A1	20060517	EP 2004-763813		20040805
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
US 2005101614	A1	20050512	US 2004-916073		20040811
PRIORITY APPLN. INFO.:			US 2003-495179P	P	20030814
			US 2004-574384P	P	20040525
			WO 2004-EP8767	W	20040805

OTHER SOURCE(S): MARPAT 142:261532
GI

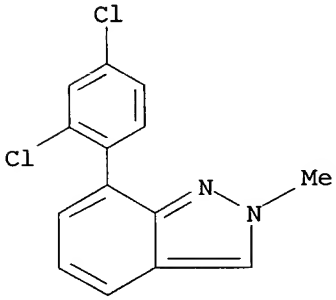


I

AB Title compds. I [R1 = alkynyl, haloalkyl, halo, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = (un)substituted aryl, (un)substituted heteroaryl with alkyl, alkoxy, alkylthio, etc.; R4 = alkyl, alkoxy, haloalkyl, etc.; n = 0-p, where p = 3 minus the number of A1, A2 and A3 which are nitrogen; A1, A2, A3 = C, N with the proviso that at least one of A1, A2 and A3 is CH or CR4] and their pharmaceutically acceptable salts were prepared For example, bromination of 7-(2,4-dichlorophenyl)-2-methyl-2H-indazole afforded 3-bromo-7-(2,4-dichlorophenyl)-2-methyl-2H-indazole (II) in 62% yield. The exemplified compound II was tested in GABAA $\alpha 1\beta 2\gamma 2$ binding assay, exhibited the pIC50 value of 6.24. Compds. I are claimed useful for the treatment of depression, convulsive disorder, etc. Formulations are given.

IT **701910-15-8P 701910-17-0P 701910-35-2P 845751-52-2P 845751-55-5P 845751-68-0P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzoindazole compds. as gabanergic modulators for treatment of depression, convulsive disorder, etc.)

RN 701910-15-8 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



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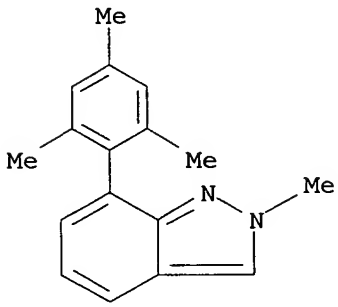
CN 2H-Indazole, 2-methyl-7-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



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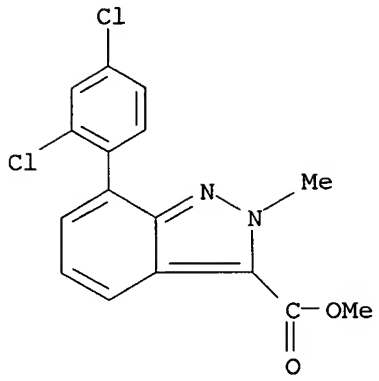
CN 2H-Indazole-3-carboxylic acid, 7-(2,4-dichlorophenyl)-2-methyl-, methyl

ester (9CI) (CA INDEX NAME)



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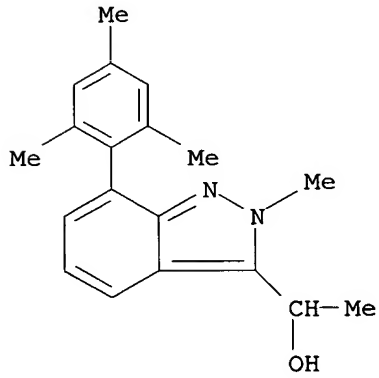

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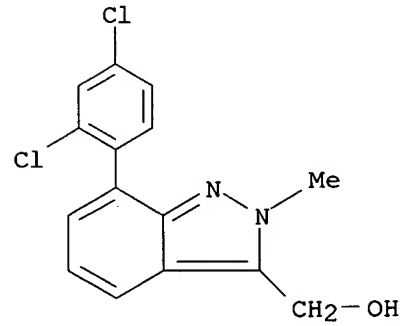

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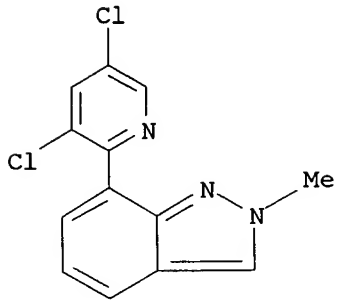

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845750-57-4P 845750-58-5P 845750-59-6P
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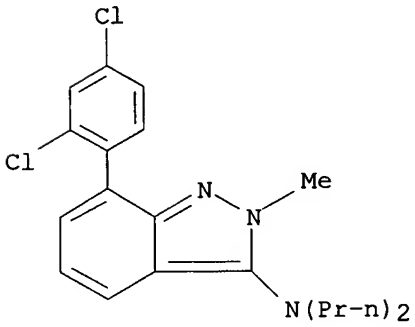
845751-85-1P 845751-89-5P 845751-99-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoindazole compds. as gabanergic modulators for treatment of depression, convulsive disorder, etc.)

RN 701909-70-8 CAPLUS
CN 2H-Indazol-3-amine, 7-(2,4-dichlorophenyl)-2-methyl-N,N-dipropyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

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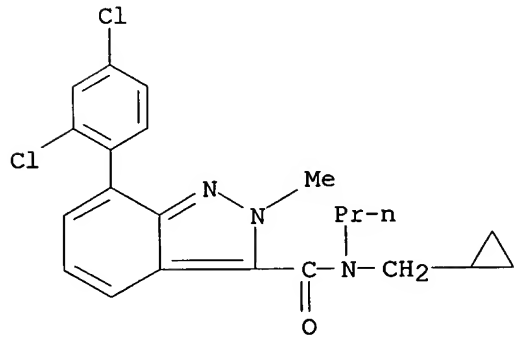
CN 2H-Indazole-3-carboxamide, N-(cyclopropylmethyl)-7-(2,4-dichlorophenyl)-2-methyl-N-propyl- (9CI) (CA INDEX NAME)



RN 701909-95-7 CAPLUS
CN 2H-Indazole-3-carboxamide, 7-(2,4-dichlorophenyl)-N,N-bis(2-methoxyethyl)-2-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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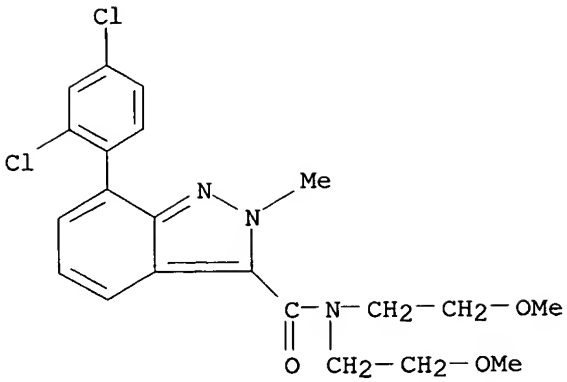
CRN 701909-94-6
CMF C21 H23 Cl2 N3 O3



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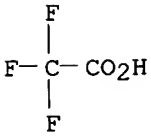
CRN 76-05-1
CMF C2 H F3 O2



RN 701910-08-9 CAPLUS
CN 2H-Indazole-3-carboxamide, 7-(2,4-dichlorophenyl)-N,N-diethyl-2-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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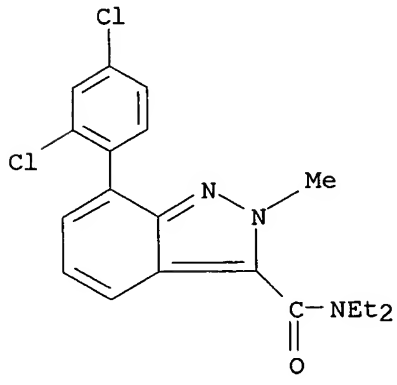
CRN 701910-07-8
CMF C19 H19 Cl2 N3 O



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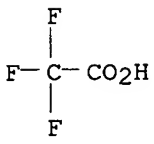
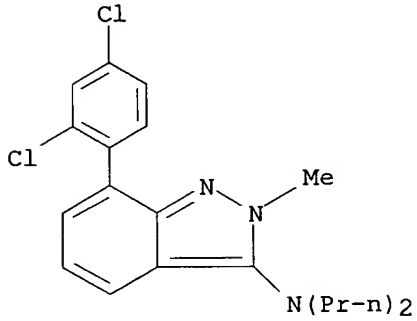
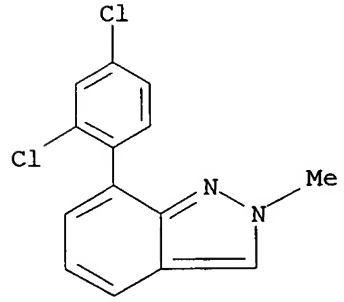
CRN 76-05-1
CMF C2 H F3 O2



RN 701910-42-1 CAPLUS
CN 2H-Indazol-3-amine, 7-(2,4-dichlorophenyl)-2-methyl-N,N-dipropyl- (9CI) (CA INDEX NAME)



RN 845750-43-8 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 845750-45-0 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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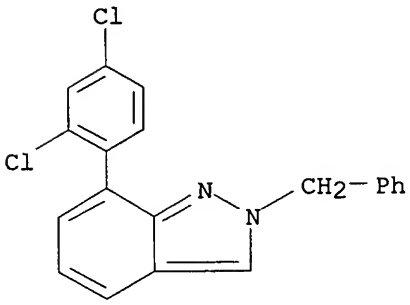
CRN 845750-44-9
CMF C20 H14 Cl2 N2



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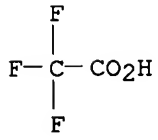
CRN 76-05-1
CMF C2 H F3 O2



RN 845750-47-2 CAPLUS
CN 2H-Indazole-2-acetic acid, 7-(2,4-dichlorophenyl)-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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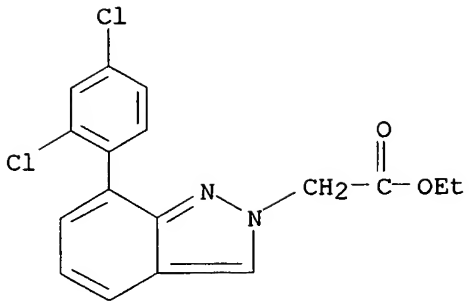
CRN 845750-46-1
CMF C17 H14 Cl2 N2 O2



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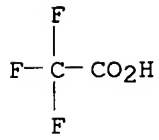

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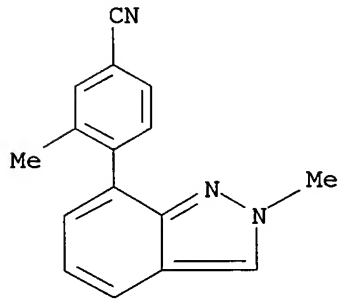
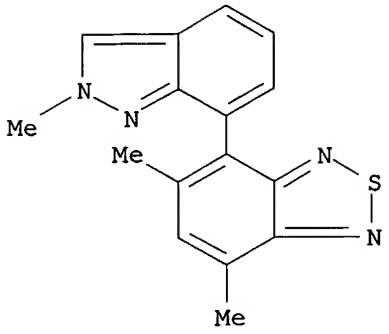
CN Benzonitrile, 3-methyl-4-(2-methyl-2H-indazol-7-yl)- (9CI) (CA INDEX NAME)



RN 845750-49-4 CAPLUS
CN 2,1,3-Benzothiadiazole, 5,7-dimethyl-4-(2-methyl-2H-indazol-7-yl)- (9CI) (CA INDEX NAME)



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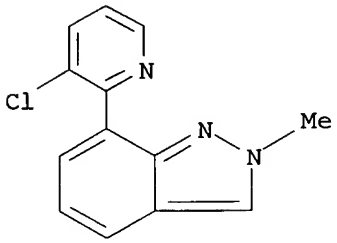

RN 845750-52-9 CAPLUS
CN 2H-Indazole, 2-methyl-7-phenyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 845750-51-8
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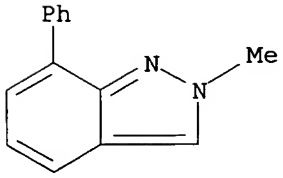

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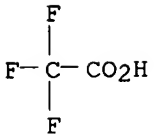

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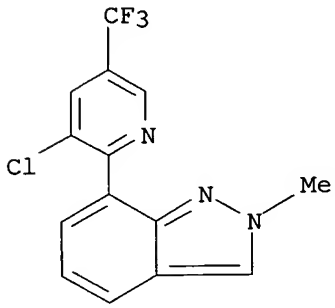

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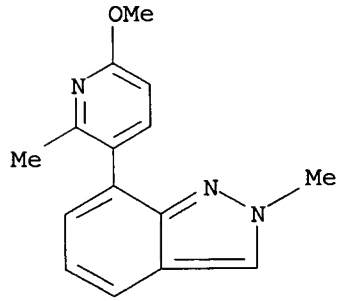

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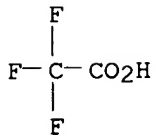

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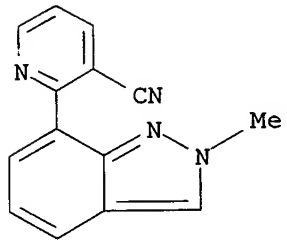
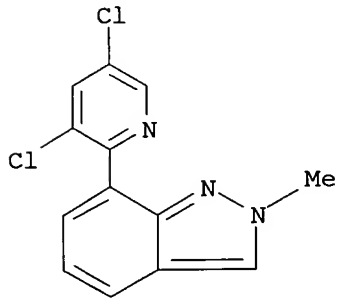
CN 3-Pyridinecarbonitrile, 2-(2-methyl-2H-indazol-7-yl)- (9CI) (CA INDEX NAME)

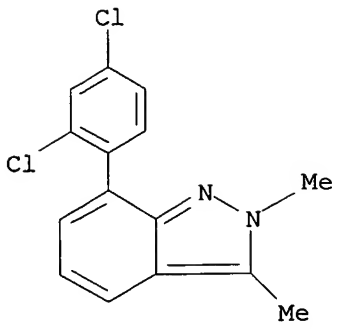


RN 845750-57-4 CAPLUS
CN 2H-Indazole, 7-(3,5-dichloro-2-pyridinyl)-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



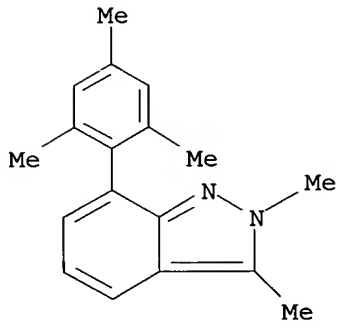
● HCl

RN 845750-58-5 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2,3-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 845750-59-6 CAPLUS
CN 2H-Indazole, 2,3-dimethyl-7-(2,4,6-trimethylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

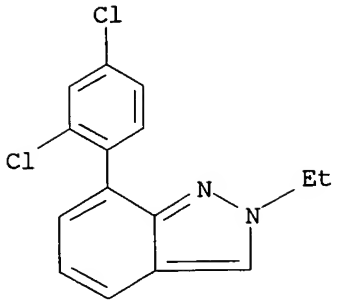


● HCl

RN 845750-61-0 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-ethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

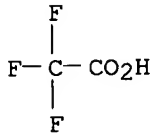
CM 1

CRN 845750-60-9
CMF C15 H12 Cl2 N2

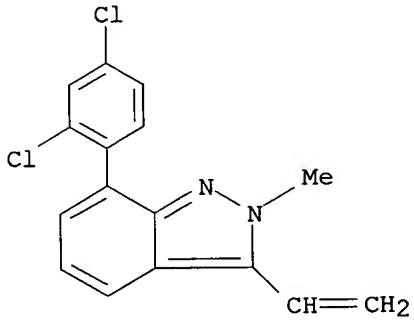


CM 2

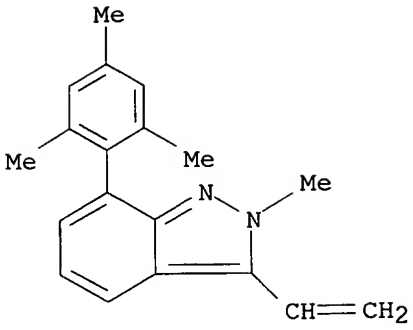
CRN 76-05-1
CMF C2 H F3 O2



RN 845750-62-1 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-3-ethenyl-2-methyl- (9CI) (CA INDEX NAME)

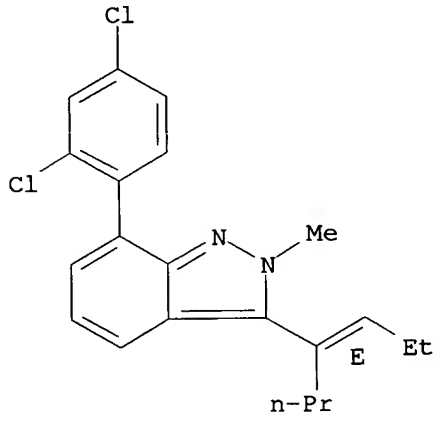


RN 845750-63-2 CAPLUS
CN 2H-Indazole, 3-ethenyl-2-methyl-7-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



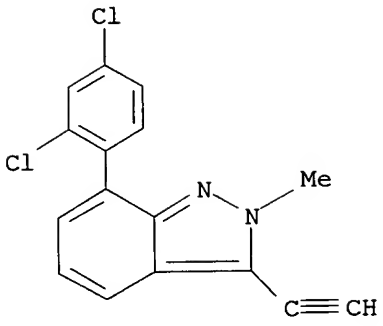
RN 845750-64-3 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-methyl-3-[(1E)-1-propyl-1-butenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Double bond geometry as shown.

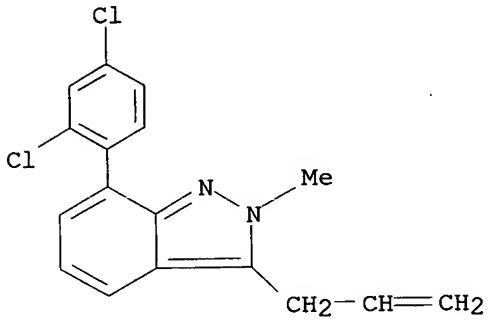


● HCl

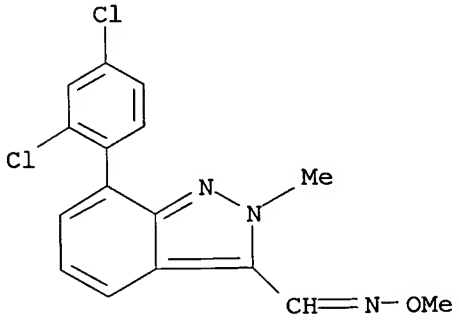
RN 845750-65-4 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-3-ethynyl-2-methyl- (9CI) (CA INDEX NAME)



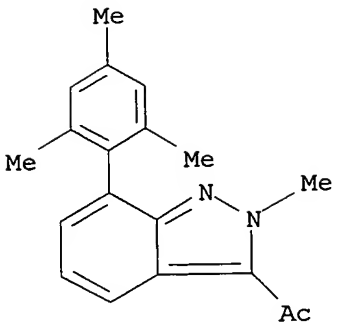
RN 845750-66-5 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-methyl-3-(2-propenyl)- (9CI) (CA INDEX NAME)



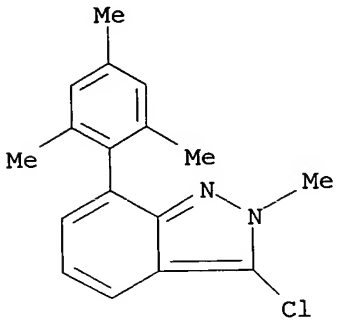
RN 845750-67-6 CAPLUS
CN 2H-Indazole-3-carboxaldehyde, 7-(2,4-dichlorophenyl)-2-methyl-, O-methyloxime (9CI) (CA INDEX NAME)



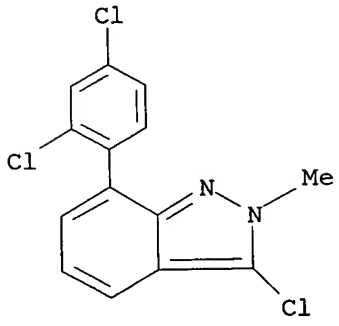
RN 845750-68-7 CAPLUS
CN Ethanone, 1-[2-methyl-7-(2,4,6-trimethylphenyl)-2H-indazol-3-yl]- (9CI) (CA INDEX NAME)



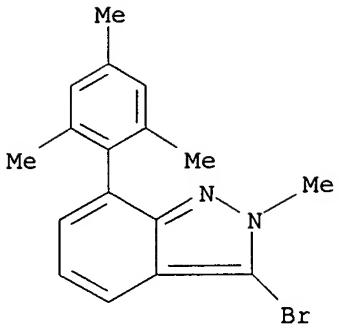
RN 845750-69-8 CAPLUS
CN 2H-Indazole, 3-chloro-2-methyl-7-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



RN 845750-70-1 CAPLUS
CN 2H-Indazole, 3-chloro-7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)

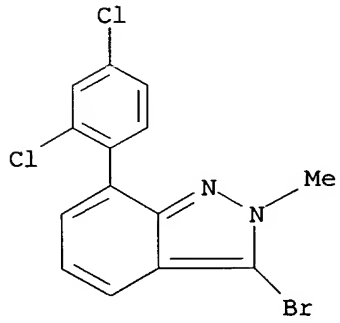


RN 845750-71-2 CAPLUS
CN 2H-Indazole, 3-bromo-2-methyl-7-(2,4,6-trimethylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

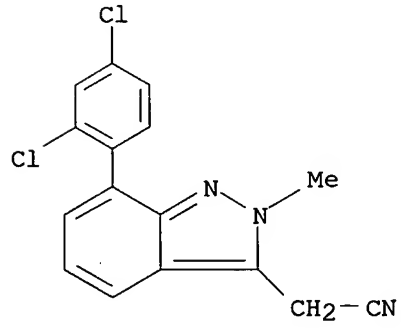


● HCl

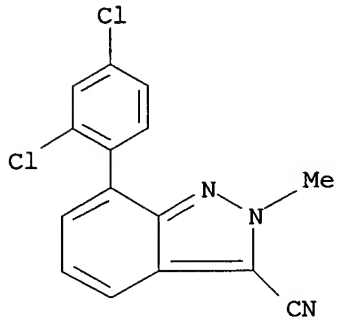
RN 845750-72-3 CAPLUS
CN 2H-Indazole, 3-bromo-7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



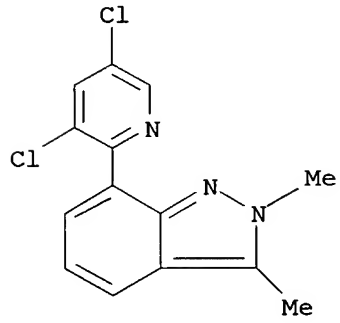
RN 845750-73-4 CAPLUS
CN 2H-Indazole-3-acetonitrile, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



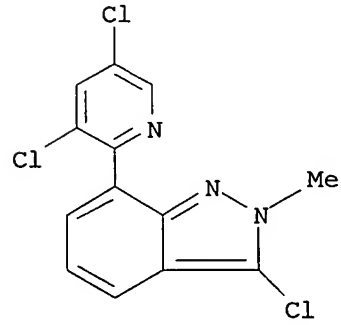
RN 845750-74-5 CAPLUS
CN 2H-Indazole-3-carbonitrile, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



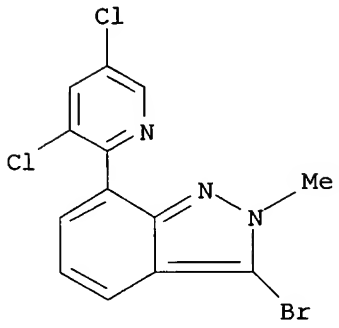
RN 845750-75-6 CAPLUS
CN 2H-Indazole, 7-(3,5-dichloro-2-pyridinyl)-2,3-dimethyl- (9CI) (CA INDEX NAME)



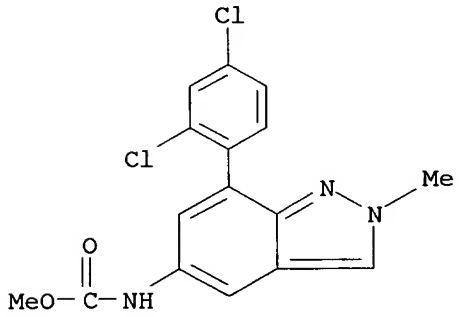
RN 845750-76-7 CAPLUS
CN 2H-Indazole, 3-chloro-7-(3,5-dichloro-2-pyridinyl)-2-methyl- (9CI) (CA INDEX NAME)



RN 845750-77-8 CAPLUS
CN 2H-Indazole, 3-bromo-7-(3,5-dichloro-2-pyridinyl)-2-methyl- (9CI) (CA INDEX NAME)

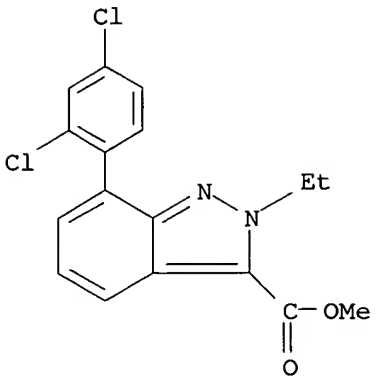


RN 845750-81-4 CAPLUS
CN Carbamic acid, [7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-5-yl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

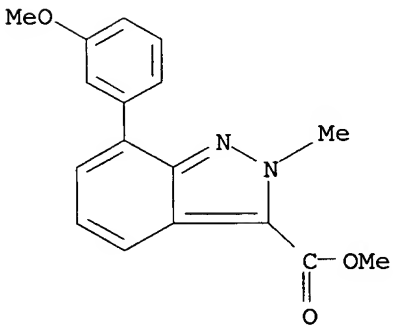
RN 845750-82-5 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(2,4-dichlorophenyl)-2-ethyl-, methyl ester (9CI) (CA INDEX NAME)



RN 845750-84-7 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(3-methoxyphenyl)-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

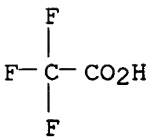
CM 1

CRN 845750-83-6
CMF C17 H16 N2 O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

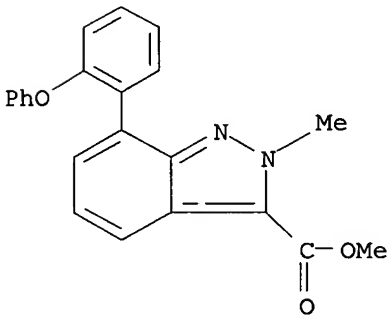


RN 845750-86-9 CAPLUS

CN 2H-Indazole-3-carboxylic acid, 2-methyl-7-(2-phenoxyphenyl)-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

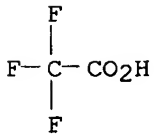
CM 1

CRN 845750-85-8
CMF C22 H18 N2 O3



CM 2

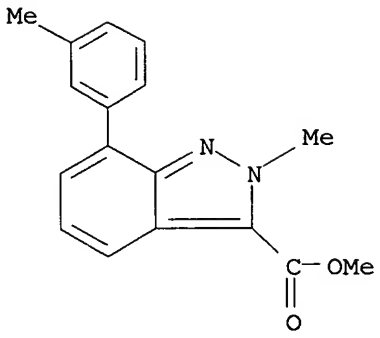
CRN 76-05-1
CMF C2 H F3 O2



RN 845750-88-1 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 2-methyl-7-(3-methylphenyl)-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

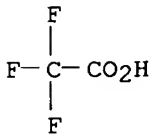
CM 1

CRN 845750-87-0
CMF C17 H16 N2 O2



CM 2

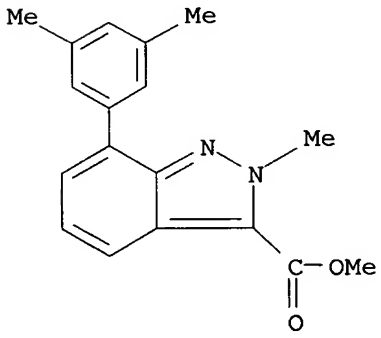
CRN 76-05-1
CMF C2 H F3 O2



RN 845750-90-5 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(3,5-dimethylphenyl)-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

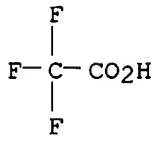
CM 1

CRN 845750-89-2
CMF C18 H18 N2 O2



CM 2

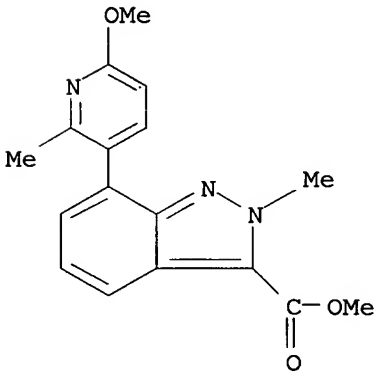
CRN 76-05-1
CMF C2 H F3 O2



RN 845750-92-7 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(6-methoxy-2-methyl-3-pyridinyl)-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

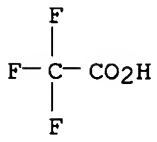
CM 1

CRN 845750-91-6
CMF C17 H17 N3 O3



CM 2

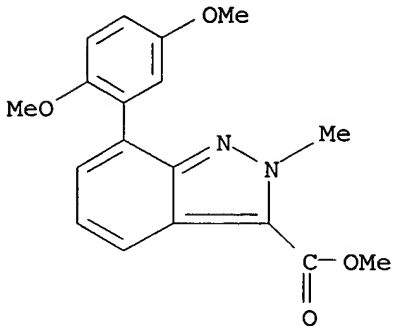
CRN 76-05-1
CMF C2 H F3 O2



RN 845750-94-9 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(2,5-dimethoxyphenyl)-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

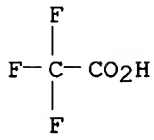
CM 1

CRN 845750-93-8
CMF C18 H18 N2 O4



CM 2

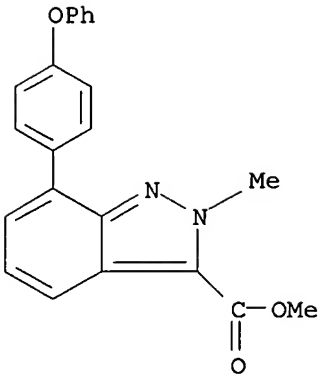
CRN 76-05-1
CMF C2 H F3 O2



RN 845750-96-1 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 2-methyl-7-(4-phenoxyphenyl)-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

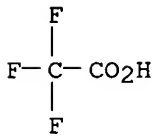
CM 1

CRN 845750-95-0
CMF C22 H18 N2 O3



CM 2

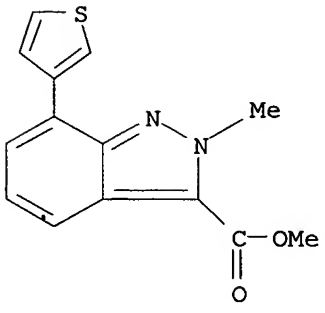
CRN 76-05-1
CMF C2 H F3 O2



RN 845750-98-3 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 2-methyl-7-(3-thienyl)-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

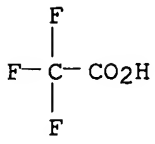
CM 1

CRN 845750-97-2
CMF C14 H12 N2 O2 S



CM 2

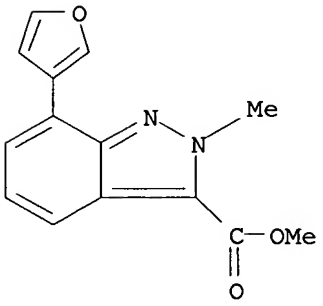
CRN 76-05-1
CMF C2 H F3 O2



RN 845751-00-0 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(3-furanyl)-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

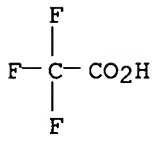
CM 1

CRN 845750-99-4
CMF C14 H12 N2 O3



CM 2

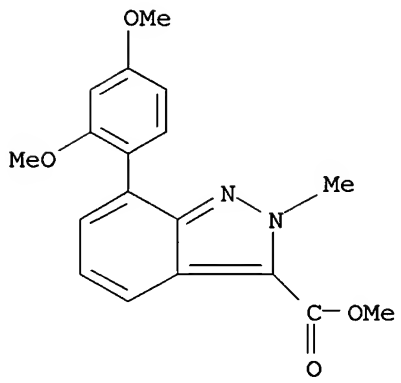
CRN 76-05-1
CMF C2 H F3 O2



RN 845751-02-2 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(2,4-dimethoxyphenyl)-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

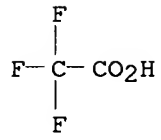
CM 1

CRN 845751-01-1
CMF C18 H18 N2 O4



CM 2

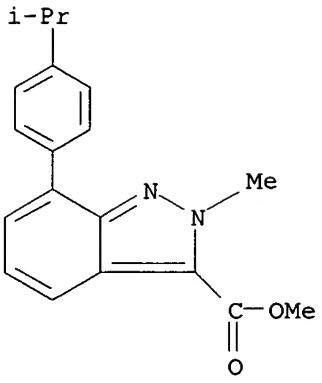
CRN 76-05-1
CMF C2 H F3 O2



RN 845751-04-4 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 2-methyl-7-[4-(1-methylethyl)phenyl]-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

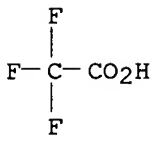
CM 1

CRN 845751-03-3
CMF C19 H20 N2 O2



CM 2

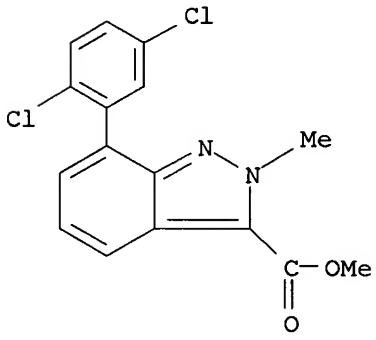
CRN 76-05-1
CMF C2 H F3 O2



RN 845751-06-6 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(2,5-dichlorophenyl)-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

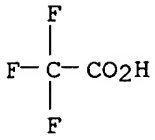
CM 1

CRN 845751-05-5
CMF C16 H12 Cl2 N2 O2



CM 2

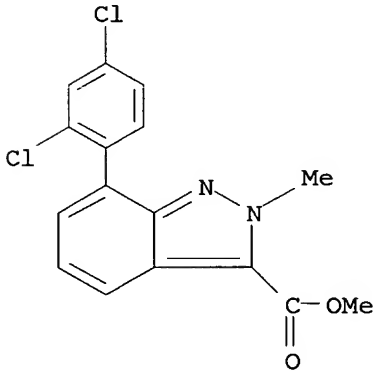
CRN 76-05-1
CMF C2 H F3 O2



RN 845751-07-7 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(2,4-dichlorophenyl)-2-methyl-, methyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

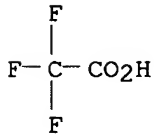
CM 1

CRN 701910-35-2
CMF C16 H12 Cl2 N2 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2

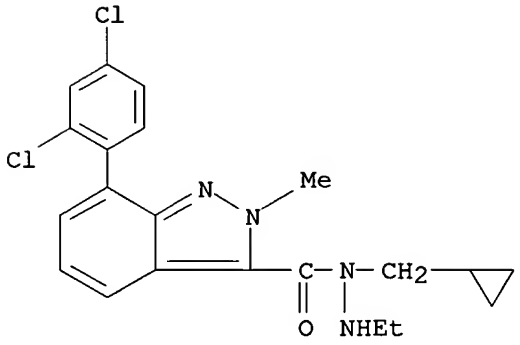


RN 845751-09-9 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(2,4-dichlorophenyl)-2-methyl-,

1-(cyclopropylmethyl)-2-ethylhydrazide, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

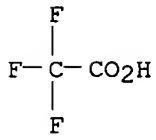
CM 1

CRN 845751-08-8
CMF C21 H22 Cl2 N4 O



CM 2

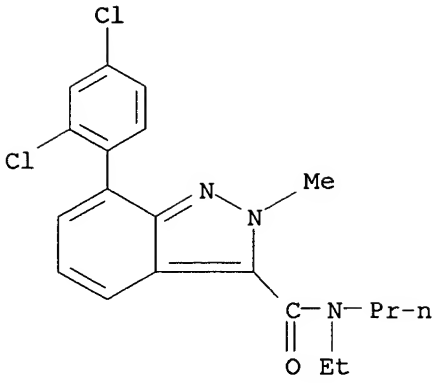
CRN 76-05-1
CMF C2 H F3 O2



RN 845751-11-3 CAPLUS
CN 2H-Indazole-3-carboxamide, 7-(2,4-dichlorophenyl)-N-ethyl-2-methyl-N-propyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

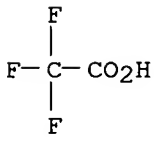
CM 1

CRN 845751-10-2
CMF C20 H21 Cl2 N3 O



CM 2

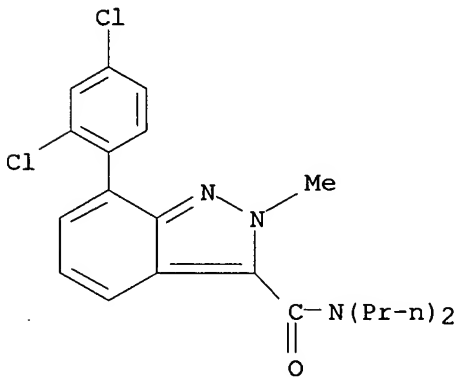
CRN 76-05-1
CMF C2 H F3 O2



RN 845751-13-5 CAPLUS
CN 2H-Indazole-3-carboxamide, 7-(2,4-dichlorophenyl)-2-methyl-N,N-dipropyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

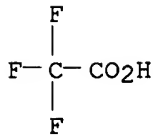
CM 1

CRN 845751-12-4
CMF C21 H23 Cl2 N3 O



CM 2

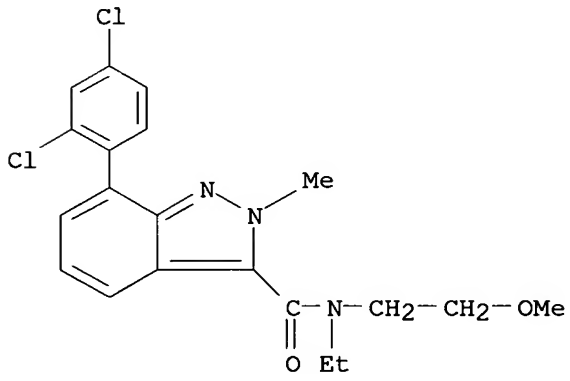
CRN 76-05-1
CMF C2 H F3 O2



RN 845751-15-7 CAPLUS
CN 2H-Indazole-3-carboxamide, 7-(2,4-dichlorophenyl)-N-ethyl-N-(2-methoxyethyl)-2-methyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

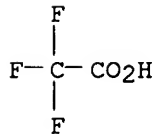
CM 1

CRN 845751-14-6
CMF C20 H21 Cl2 N3 O2



CM 2

CRN 76-05-1
CMF C2 H F3 O2

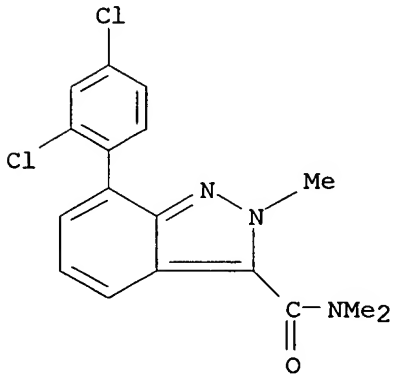


RN 845751-17-9 CAPLUS

CN 2H-Indazole-3-carboxamide, 7-(2,4-dichlorophenyl)-N,N,2-trimethyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

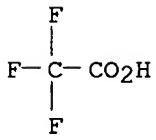
CM 1

CRN 845751-16-8
CMF C17 H15 Cl2 N3 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2

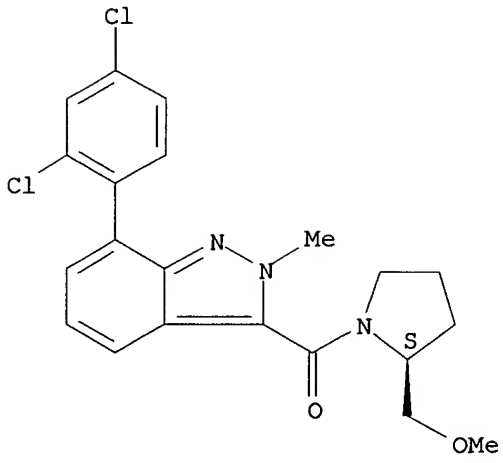


RN 845751-19-1 CAPLUS
CN Pyrrolidine, 1-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]carbonyl]-2-(methoxymethyl)-, (2S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

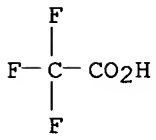
CRN 845751-18-0
CMF C21 H21 Cl2 N3 O2

Absolute stereochemistry.

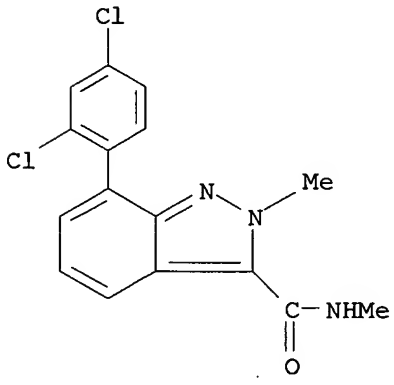


CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 845751-20-4 CAPLUS
CN 2H-Indazole-3-carboxamide, 7-(2,4-dichlorophenyl)-N,2-dimethyl- (9CI) (CA INDEX NAME)

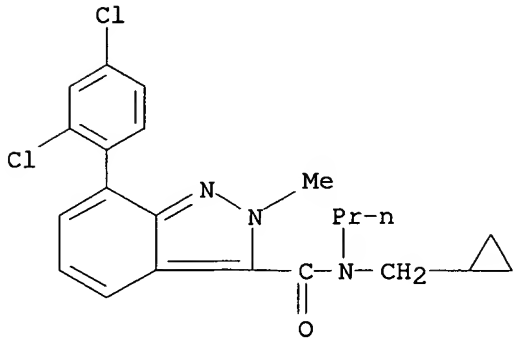


RN 845751-21-5 CAPLUS
CN 2H-Indazole-3-carboxamide, N-(cyclopropylmethyl)-7-(2,4-dichlorophenyl)-2-

methyl-N-propyl-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

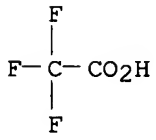
CM 1

CRN 701909-88-8
CMF C22 H23 Cl2 N3 O

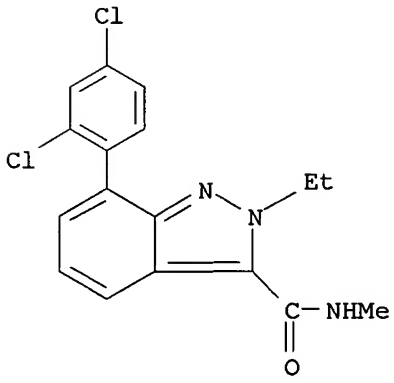


CM 2

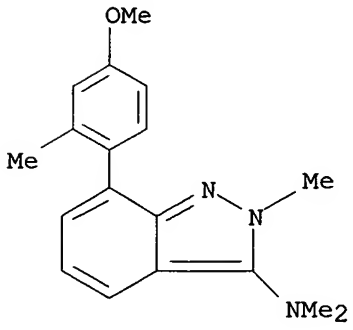
CRN 76-05-1
CMF C2 H F3 O2



RN 845751-22-6 CAPLUS
CN 2H-Indazole-3-carboxamide, 7-(2,4-dichlorophenyl)-2-ethyl-N-methyl- (9CI) (CA INDEX NAME)

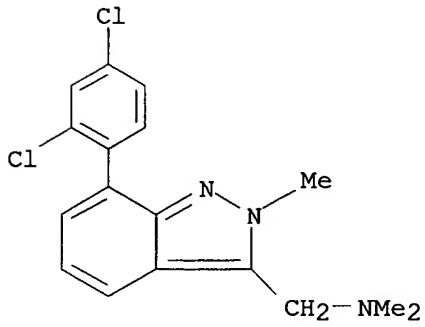


RN 845751-23-7 CAPLUS
CN 2H-Indazol-3-amine, 7-(4-methoxy-2-methylphenyl)-N,N,2-trimethyl-, monohydrochloride (9CI) (CA INDEX NAME)

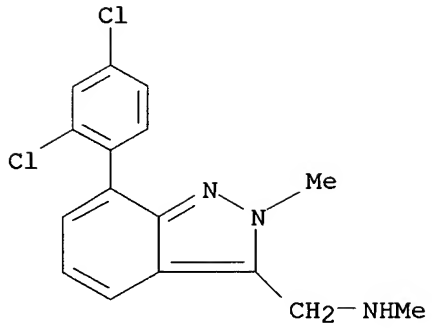


● HCl

RN 845751-24-8 CAPLUS
CN 2H-Indazole-3-methanamine, 7-(2,4-dichlorophenyl)-N,N,2-trimethyl- (9CI) (CA INDEX NAME)

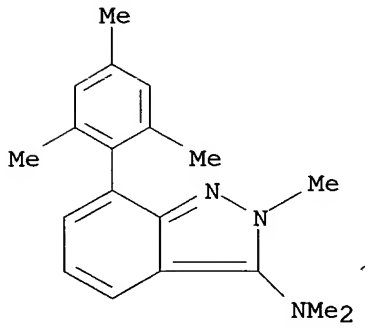


RN 845751-25-9 CAPLUS
CN 2H-Indazole-3-methanamine, 7-(2,4-dichlorophenyl)-N,2-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



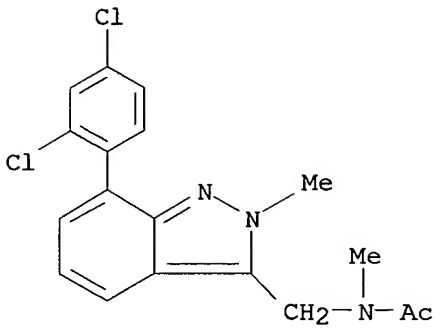
● HCl

RN 845751-26-0 CAPLUS
CN 2H-Indazol-3-amine, N,N,2-trimethyl-7-(2,4,6-trimethylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)



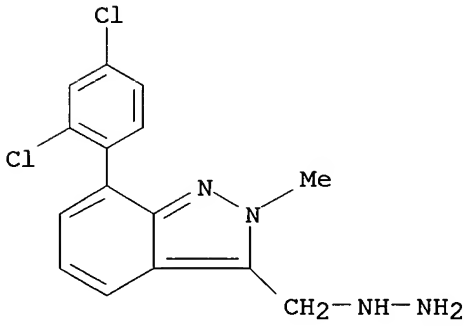
● HCl

RN 845751-27-1 CAPLUS
CN Acetamide, N-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]methyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



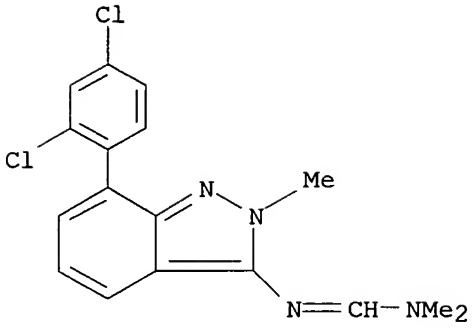
● HCl

RN 845751-28-2 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-3-(hydrazinomethyl)-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



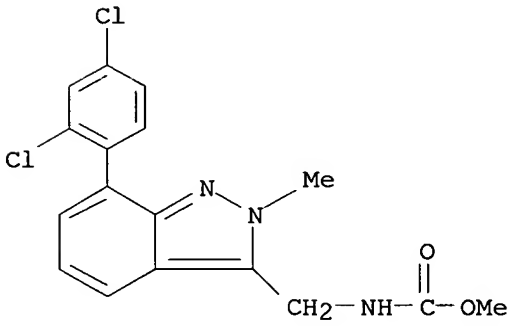
● HCl

RN 845751-29-3 CAPLUS
CN Methanimidamide, N'-[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]-N,N-dimethyl-, monohydrochloride (9CI) (CA INDEX NAME)



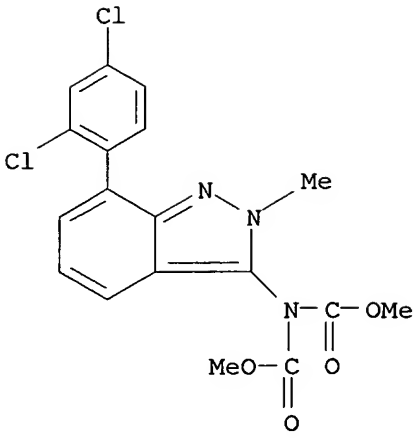
● HCl

RN 845751-30-6 CAPLUS
CN Carbamic acid, [[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]methyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



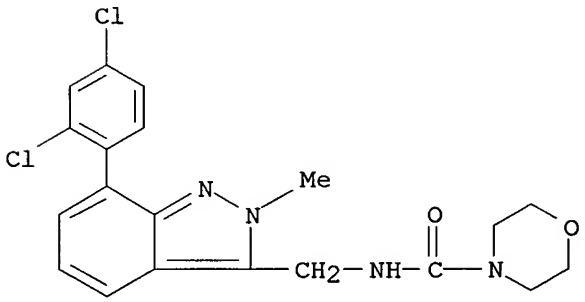
● HCl

RN 845751-31-7 CAPLUS
CN Imidodicarbonic acid, [7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]-, dimethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

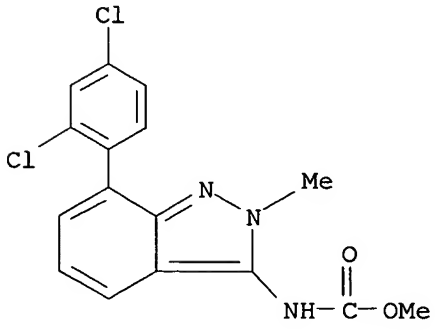


● HCl

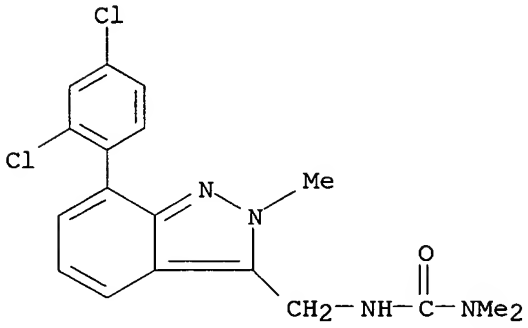
RN 845751-32-8 CAPLUS
CN 4-Morpholinecarboxamide, N-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]methyl]- (9CI) (CA INDEX NAME)



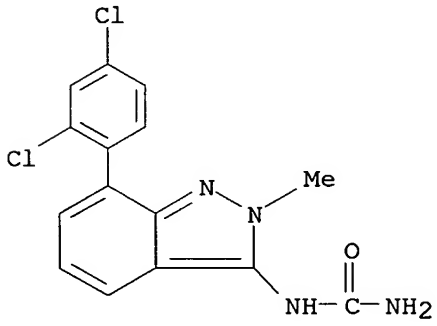
RN 845751-33-9 CAPLUS
CN Carbamic acid, [7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]-, methyl ester (9CI) (CA INDEX NAME)



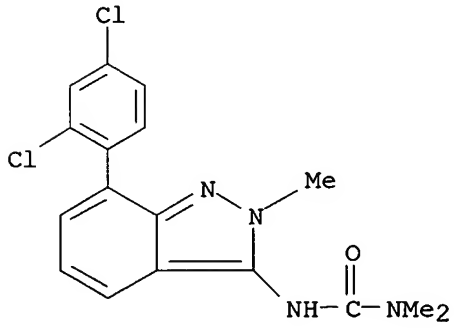
RN 845751-34-0 CAPLUS
CN Urea, N'-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



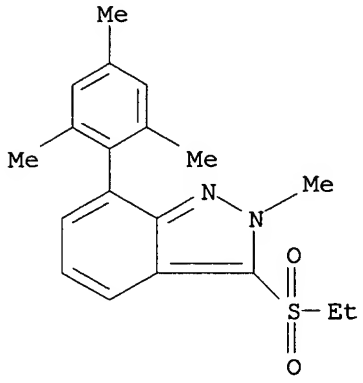
RN 845751-35-1 CAPLUS
CN Urea, [7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]- (9CI) (CA INDEX NAME)



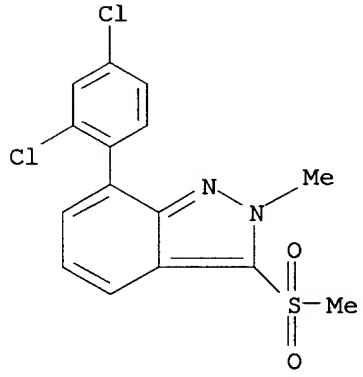
RN 845751-36-2 CAPLUS
CN Urea, N'-[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



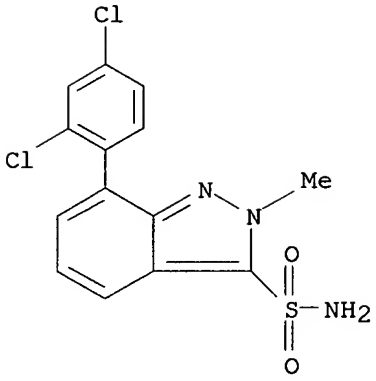
RN 845751-37-3 CAPLUS
CN 2H-Indazole, 3-(ethylsulfonyl)-2-methyl-7-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



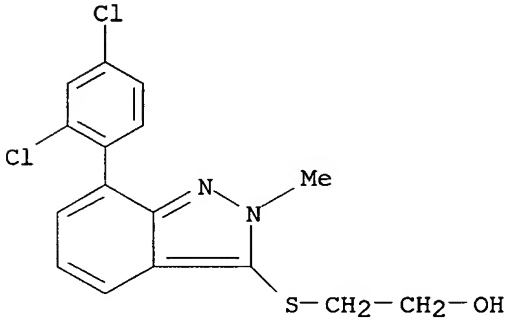
RN 845751-38-4 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-methyl-3-(methylsulfonyl)- (9CI) (CA INDEX NAME)



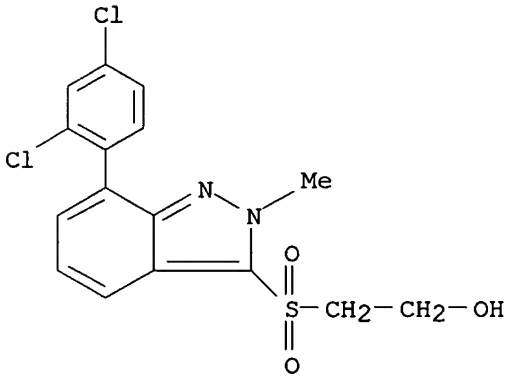
RN 845751-39-5 CAPLUS
CN 2H-Indazole-3-sulfonamide, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



RN 845751-40-8 CAPLUS
CN Ethanol, 2-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]thio]- (9CI) (CA INDEX NAME)

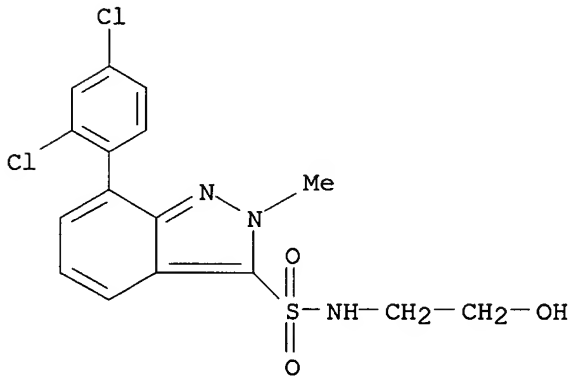


RN 845751-41-9 CAPLUS
CN Ethanol, 2-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]sulfonyl]- (9CI) (CA INDEX NAME)

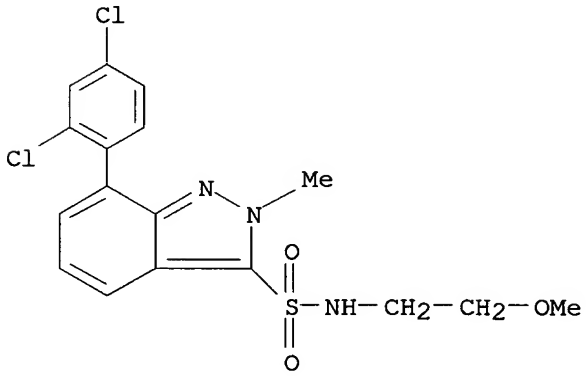


RN 845751-42-0 CAPLUS

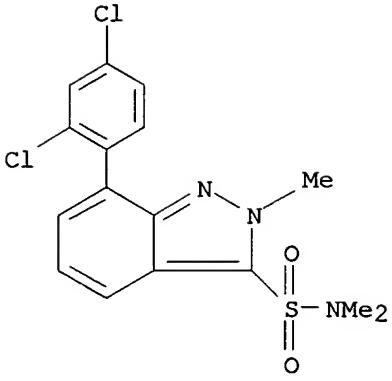
CN 2H-Indazole-3-sulfonamide, 7-(2,4-dichlorophenyl)-N-(2-hydroxyethyl)-2-methyl- (9CI) (CA INDEX NAME)



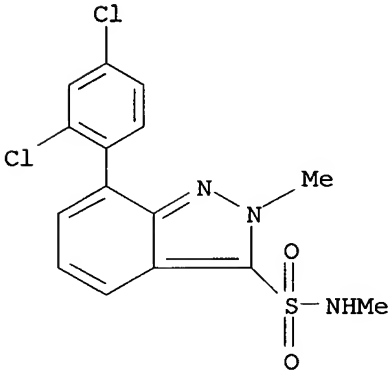
RN 845751-43-1 CAPLUS
CN 2H-Indazole-3-sulfonamide, 7-(2,4-dichlorophenyl)-N-(2-methoxyethyl)-2-methyl- (9CI) (CA INDEX NAME)



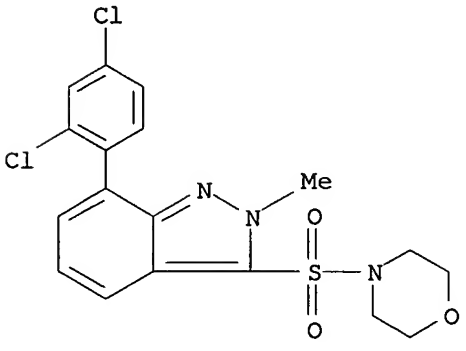
RN 845751-44-2 CAPLUS
CN 2H-Indazole-3-sulfonamide, 7-(2,4-dichlorophenyl)-N,N,2-trimethyl- (9CI) (CA INDEX NAME)



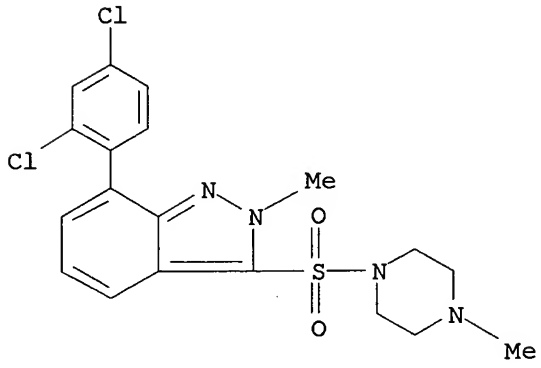
RN 845751-45-3 CAPLUS
CN 2H-Indazole-3-sulfonamide, 7-(2,4-dichlorophenyl)-N,2-dimethyl- (9CI) (CA INDEX NAME)



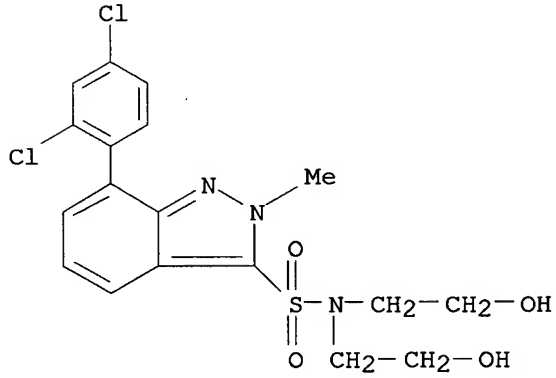
RN 845751-46-4 CAPLUS
CN Morpholine, 4-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]sulfonyl]- (9CI) (CA INDEX NAME)



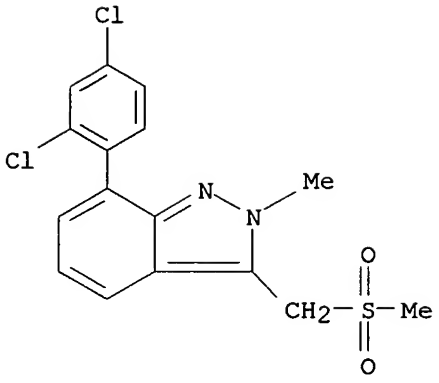
RN 845751-47-5 CAPLUS
CN Piperazine, 1-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]sulfonyl]-4-methyl- (9CI) (CA INDEX NAME)



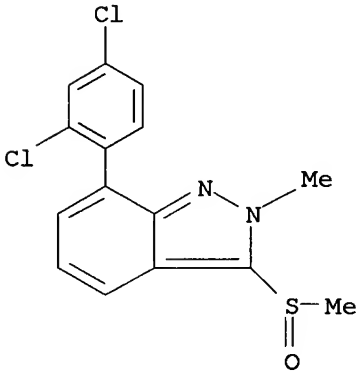
RN 845751-48-6 CAPLUS
CN 2H-Indazole-3-sulfonamide, 7-(2,4-dichlorophenyl)-N,N-bis(2-hydroxyethyl)-2-methyl- (9CI) (CA INDEX NAME)



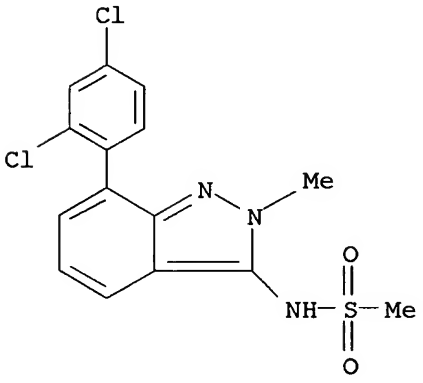
RN 845751-49-7 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-methyl-3-[(methylsulfonyl)methyl]- (9CI) (CA INDEX NAME)



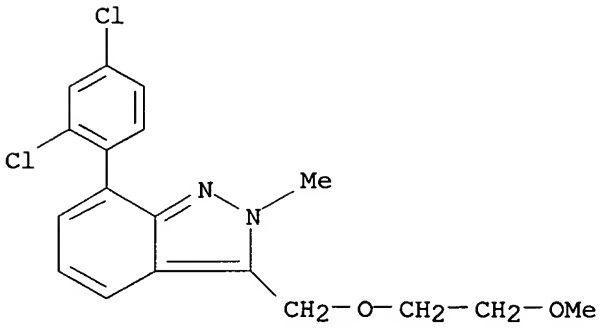
RN 845751-50-0 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-methyl-3-(methylsulfinyl)- (9CI) (CA INDEX NAME)



RN 845751-51-1 CAPLUS
CN Methanesulfonamide, N-[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]- (9CI) (CA INDEX NAME)

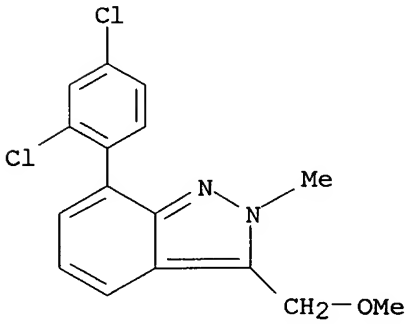


RN 845751-53-3 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-3-[(2-methoxyethoxy)methyl]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

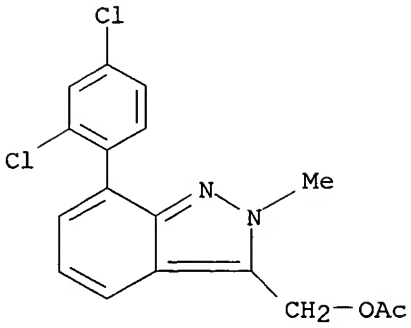


● HCl

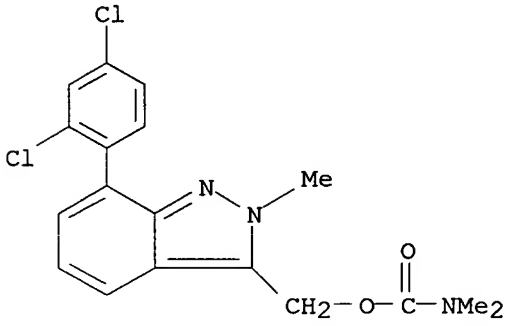
RN 845751-54-4 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-3-(methoxymethyl)-2-methyl- (9CI) (CA INDEX NAME)



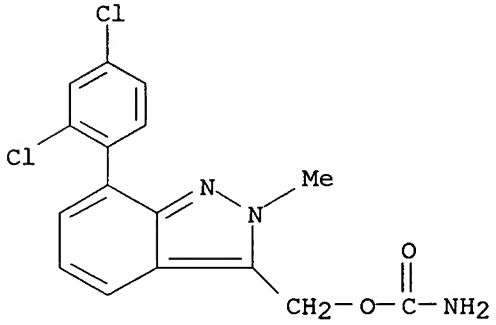
RN 845751-56-6 CAPLUS
CN 2H-Indazole-3-methanol, 7-(2,4-dichlorophenyl)-2-methyl-, acetate (ester) (9CI) (CA INDEX NAME)



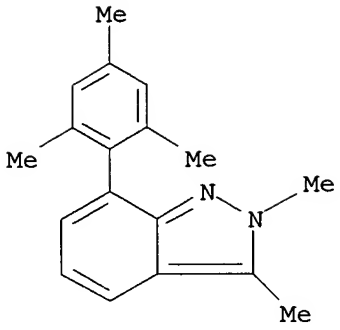
RN 845751-57-7 CAPLUS
CN Carbamic acid, dimethyl-, [7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]methyl ester (9CI) (CA INDEX NAME)



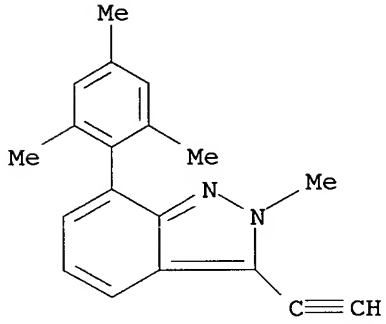
RN 845751-58-8 CAPLUS
CN 2H-Indazole-3-methanol, 7-(2,4-dichlorophenyl)-2-methyl-, carbamate (ester) (9CI) (CA INDEX NAME)



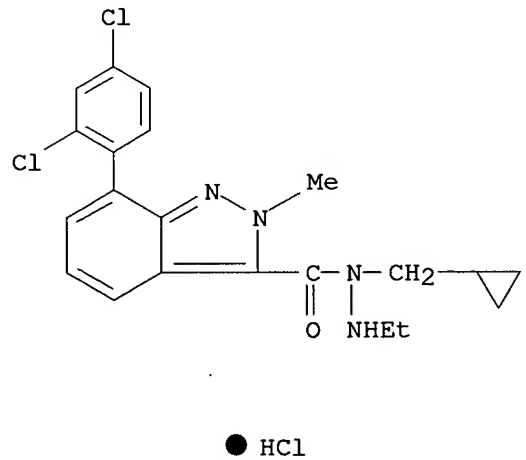
RN 845751-63-5 CAPLUS
CN 2H-Indazole, 2,3-dimethyl-7-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



RN 845751-72-6 CAPLUS
CN 2H-Indazole, 3-ethynyl-2-methyl-7-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

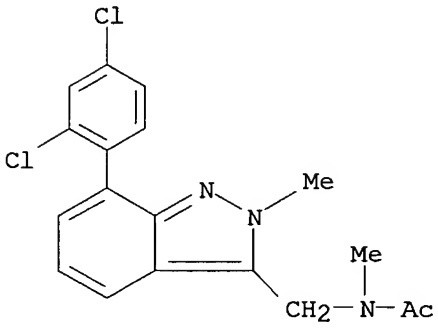


RN 845751-76-0 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(2,4-dichlorophenyl)-2-methyl-, 1-(cyclopropylmethyl)-2-ethylhydrazide, monohydrochloride (9CI) (CA INDEX NAME)

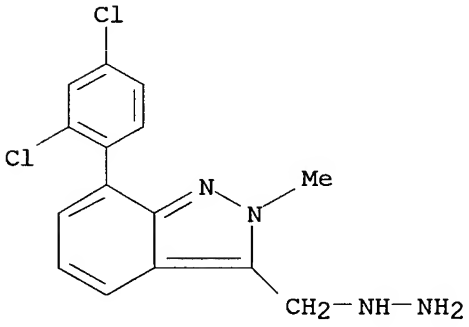


● HCl

RN 845751-85-1 CAPLUS
CN Acetamide, N-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]methyl]-N-methyl- (9CI) (CA INDEX NAME)

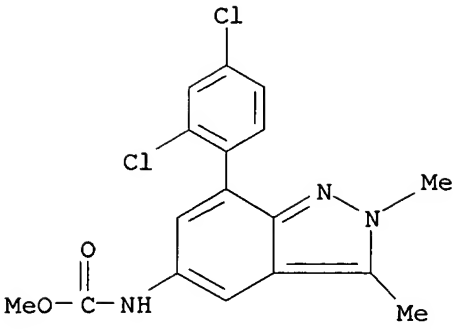


RN 845751-89-5 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-3-(hydrazinomethyl)-2-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

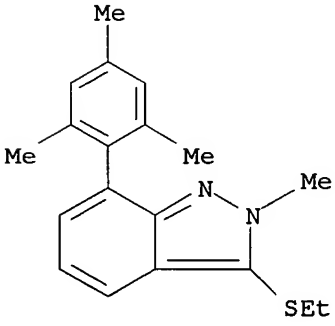
RN 845751-99-7 CAPLUS
CN Carbamic acid, [7-(2,4-dichlorophenyl)-2,3-dimethyl-2H-indazol-5-yl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)



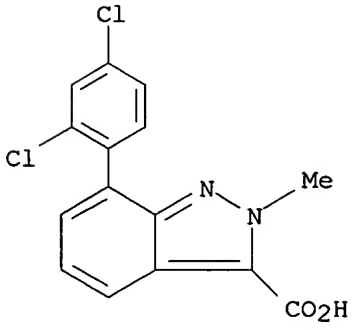
● HCl

IT **845751-74-8 845752-10-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzoindazole compds. as gabanergic modulators for treatment of depression, convulsive disorder, etc.)

RN 845751-74-8 CAPLUS
CN 2H-Indazole, 3-(ethylthio)-2-methyl-7-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)

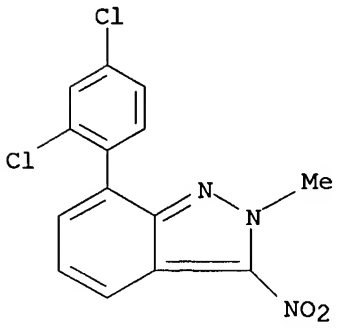


RN 845752-10-5 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)

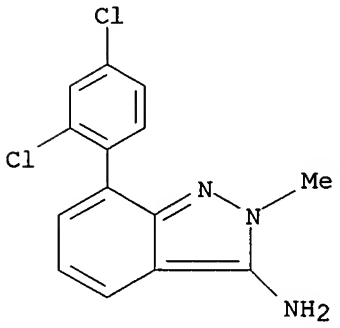


IT **701910-20-5P 701910-21-6P 701910-22-7P**
701910-23-8P 845751-71-5P 845751-77-1P
845751-83-9P 845751-84-0P 845751-86-2P
845751-87-3P 845751-88-4P 845751-90-8P
845751-95-3P 845751-96-4P 845751-97-5P
845751-98-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoindazole compds. as gabanergic modulators for treatment of depression, convulsive disorder, etc.)

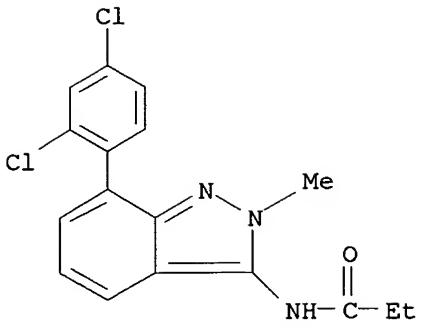
RN 701910-20-5 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-methyl-3-nitro- (9CI) (CA INDEX NAME)



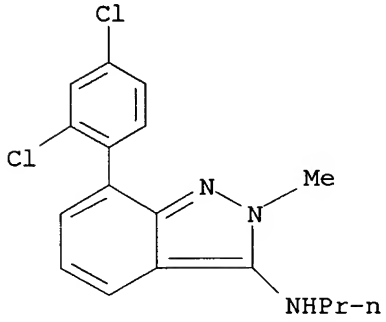
RN 701910-21-6 CAPLUS
CN 2H-Indazol-3-amine, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



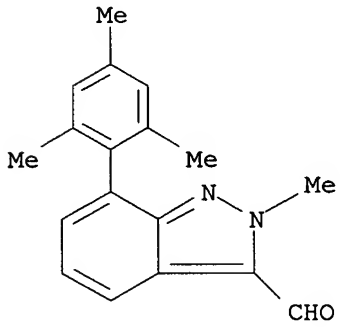
RN 701910-22-7 CAPLUS
CN Propanamide, N-[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]- (9CI) (CA INDEX NAME)



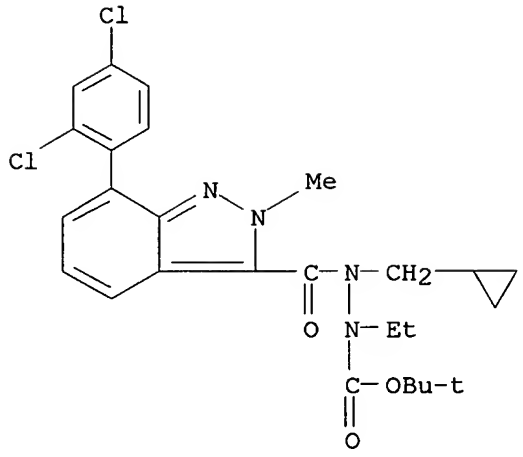
RN 701910-23-8 CAPLUS
CN 2H-Indazol-3-amine, 7-(2,4-dichlorophenyl)-2-methyl-N-propyl- (9CI) (CA INDEX NAME)



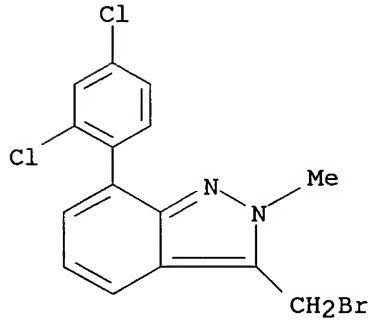
RN 845751-71-5 CAPLUS
CN 2H-Indazole-3-carboxaldehyde, 2-methyl-7-(2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



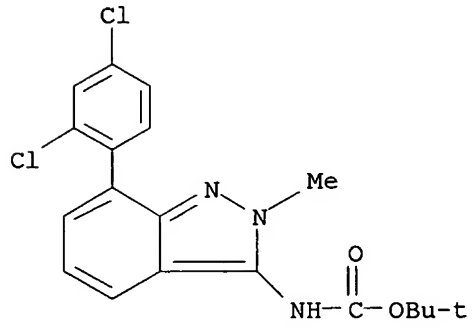
RN 845751-77-1 CAPLUS
CN 2H-Indazole-3-carboxylic acid, 7-(2,4-dichlorophenyl)-2-methyl-, 1-(cyclopropylmethyl)-2-[(1,1-dimethylethoxy)carbonyl]-2-ethylhydrazide (9CI) (CA INDEX NAME)



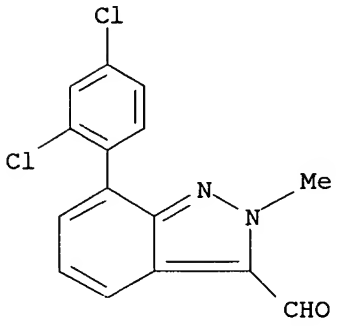
RN 845751-83-9 CAPLUS
CN 2H-Indazole, 3-(bromomethyl)-7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



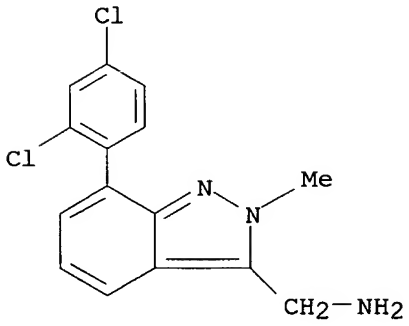
RN 845751-84-0 CAPLUS
CN Carbamic acid, [7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



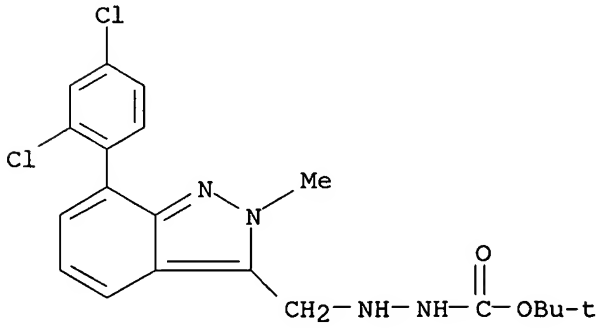
RN 845751-86-2 CAPLUS
CN 2H-Indazole-3-carboxaldehyde, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



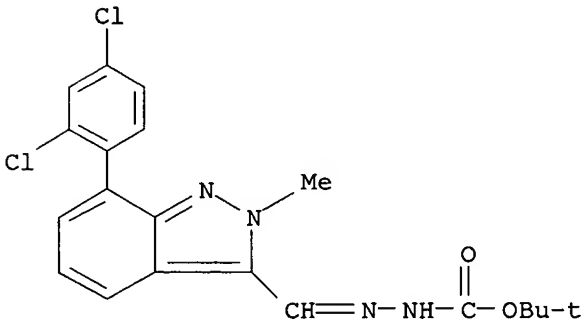
RN 845751-87-3 CAPLUS
CN 2H-Indazole-3-methanamine, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



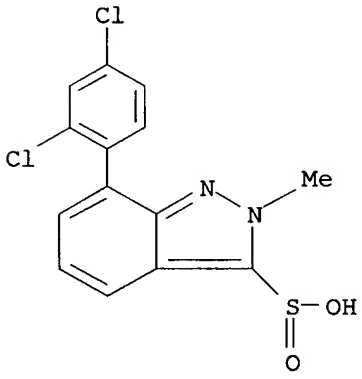
RN 845751-88-4 CAPLUS
CN Hydrazinecarboxylic acid, 2-[[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



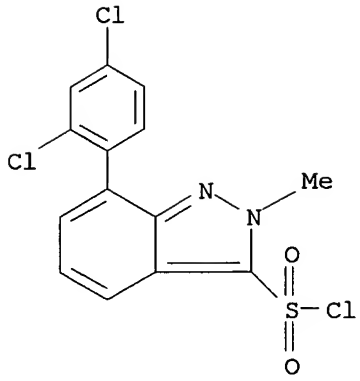
RN 845751-90-8 CAPLUS
CN Hydrazinecarboxylic acid, [[7-(2,4-dichlorophenyl)-2-methyl-2H-indazol-3-yl]methylene]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



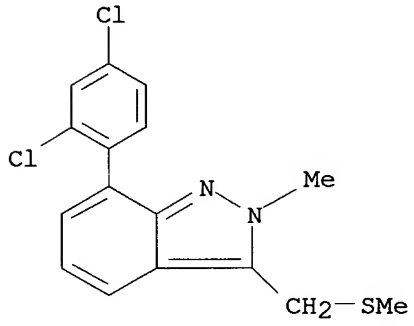
RN 845751-95-3 CAPLUS
CN 2H-Indazole-3-sulfinic acid, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



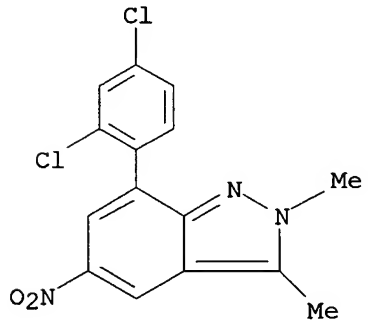
RN 845751-96-4 CAPLUS
CN 2H-Indazole-3-sulfonyl chloride, 7-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)



RN 845751-97-5 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2-methyl-3-[(methylthio)methyl]- (9CI) (CA INDEX NAME)



RN 845751-98-6 CAPLUS
CN 2H-Indazole, 7-(2,4-dichlorophenyl)-2,3-dimethyl-5-nitro- (9CI) (CA INDEX NAME)



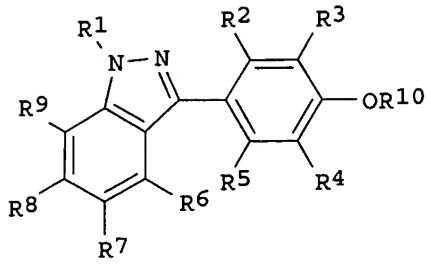
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 16 OF 30 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:308422 CAPLUS
DOCUMENT NUMBER: 140:339323
TITLE: Preparation of substituted 4-(indazol-3-yl)phenols as estrogen receptor (ER) ligands for treatment of inflammatory diseases
INVENTOR(S): Steffan, Robert John; Matelan, Edward Martin; Ashwell, Mark Anthony; Solvibile, William Ronald
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: PCT Int. Appl., 135 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

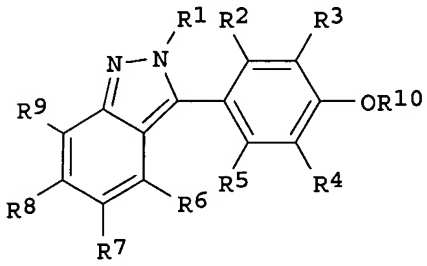
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031159	A1	20040415	WO 2003-US30252	20030924
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2499736	AA	20040415	CA 2003-2499736	20030924
AU 2003276940	A1	20040423	AU 2003-276940	20030924
US 2004167127	A1	20040826	US 2003-670646	20030924
EP 1542976	A1	20050622	EP 2003-799289	20030924
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003014475	A	20050809	BR 2003-14475	20030924
JP 2006505544	T2	20060216	JP 2004-541738	20030924
NO 2005001942	A	20050614	NO 2005-1942	20050420

PRIORITY APPLN. INFO.:		US 2002-413931P	P 20020925
		WO 2003-US30252	W 20030924

OTHER SOURCE(S): MARPAT 140:339323
GI



I



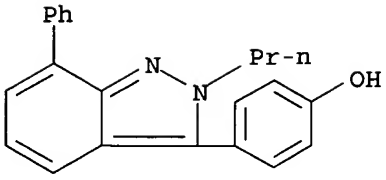
II

AB Title compds. I and II [wherein R1 = H, (cyclo)alkyl, (cyclo)alkenyl, aryl(alkyl), or heterocyclyl; R2-R5 = independently H, alkyl, alkenyl, OH, alkoxy, aryloxy, halo, CF3, CN, NO2, CHO, or CO2R11; R6-R9 = independently H, alkyl, alkenyl, OH, alkoxy, aryloxy, halo, CF3, CO2R11, aryl(alkyl), or heterocyclyl; R10 = H, COR11, CONHR11, P(O)(OH)OR11, or CO(CH2)nCH(NHR12)CO2R11; R11 = H, alkyl, or aryl(alkyl); R12 = H or CO2R11; n = 0-3; and pharmaceutically acceptable salts thereof] were prepared as antiinflammatory agents. For example, condensation of 2,2',4,4'-tetrahydroxybenzophenone with propylhydrazine•oxalate using NaOAc in MeOH provided 4-(6-hydroxy-1-propyl-1H-indazol-3-yl)benzene-1,3-diol (III). Compds. of the invention potently and efficaciously inhibited transcription factor nuclear factor κB (NF-κB) and interleukin 6 (IL-6) expression in ERα infected immortalized human aortic endothelial (HAECT-1) cells (IC50 values about 1 nM) without inducing creatinine kinase (CK) expression in an ER-dependent manner, demonstrating antiinflammatory activity in the absence of classic estrogenic activity. Thus, I, II, and their pharmaceutical compns. are useful for the treatment of the inflammatory component of diseases and are particularly useful in treating atherosclerosis, myocardial infarction, congestive heart failure, inflammatory bowel disease, arthritis, type II diabetes, and autoimmune diseases, such as multiple sclerosis and rheumatoid arthritis (no data).

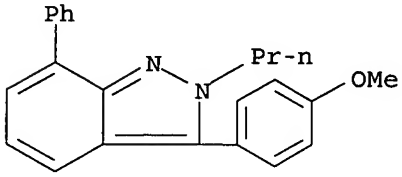
IT **680612-81-1P**, 4-(7-Phenyl-2-propyl-2H-indazol-3-yl)phenol
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(ER ligand; preparation of indazolylphenols as ER ligands for treatment of inflammatory diseases)

RN 680612-81-1 CAPLUS

CN Phenol, 4-(7-phenyl-2-propyl-2H-indazol-3-yl)- (9CI) (CA INDEX NAME)



IT **680612-82-2P**, 3-(4-Methoxyphenyl)-7-phenyl-2-propyl-2H-indazole
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of indazolylphenols as ER ligands for treatment of inflammatory diseases)
RN 680612-82-2 CAPLUS
CN 2H-Indazole, 3-(4-methoxyphenyl)-7-phenyl-2-propyl- (9CI) (CA INDEX NAME)



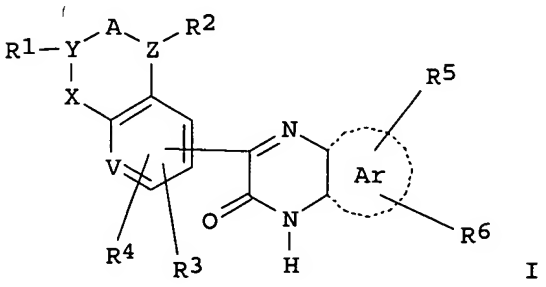
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 17 OF 43 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:31439 CAPLUS
DOCUMENT NUMBER: 136:102401
TITLE: Preparation of pyrazinone derivatives as Cdk4 and Cdk6 inhibiting anticancer agents
INVENTOR(S): Hayama, Takashi; Kawanishi, Nobuhiko; Takaki, Tooru
PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 162 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002002550	A1	20020110	WO 2001-JP5545	20010628
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001067852	A5	20020114	AU 2001-67852	20010628
CA 2413002	AA	20021219	CA 2001-2413002	20010628
EP 1295878	A1	20030326	EP 2001-945654	20010628
EP 1295878	B1	20040915		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
AT 276257	E	20041015	AT 2001-945654	20010628
ES 2223884	T3	20050301	ES 2001-1945654	20010628
US 2003203907	A1	20031030	US 2003-312500	20030131
US 6914062	B2	20050705		
US 2005176719	A1	20050811	US 2005-105534	20050414

PRIORITY APPLN. INFO.:
JP 2000-200292 A 20000630
WO 2001-JP5545 W 20010628
US 2003-312500 A3 20030131

OTHER SOURCE(S): MARPAT 136:102401
GI



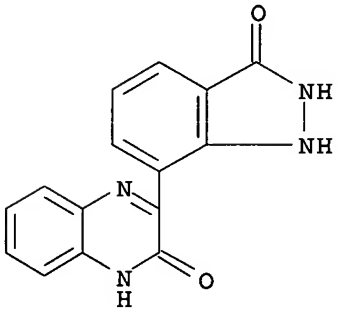
I

AB The title compds. I [A = (W)n; Ar is aryl fused to the adjacent pyrazinone

ring at its 5- and 6-positions, or the like; X is CO or the like; Y is CH or the like; Z is CH or the like; V is CH or the like; Wn is (CH2)n (wherein n is 0 to 4); R1 is hydrogen, optionally substituted lower alkyl, or the like; R2 is hydrogen or the like; R3 and R4 are each independently hydrogen or the like; and R5 and R6 are each independently hydrogen, hydroxyl, or the like] are prepared Processes for preparing I are claimed. 9-(3-Oxo-3,4-dihydroquinoxalin-2-yl)-1,2,3,9b-tetrahydro-5H-pyrrolo[2,1-a]isoindol-5-one in vitro showed IC50 of 0.3 μM against T98G cells, resp.

IT **388611-61-8P 388611-62-9P 388611-63-0P**
388611-64-1P 388612-50-8P 388612-52-0P
388612-54-2P 388612-56-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazinone derivs. as Cdk4 and Cdk6 inhibiting anticancer agents)

RN 388611-61-8 CAPLUS
CN 2(1H)-Quinoxalinone, 3-(2,3-dihydro-3-oxo-1H-indazol-7-yl)- (9CI) (CA INDEX NAME)



RN 388611-62-9 CAPLUS
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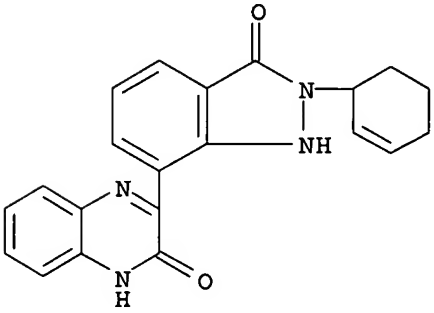
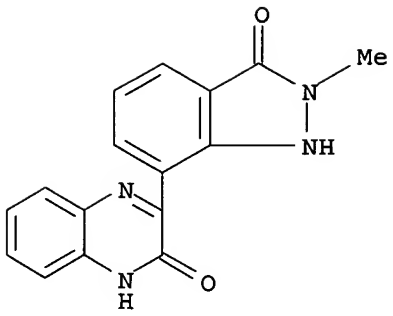


RN 388611-63-0 CAPLUS
CN 2(1H)-Quinoxalinone, 3-(2,3-dihydro-2-methyl-3-oxo-1H-indazol-7-yl)- (9CI) (CA INDEX NAME)



RN 388611-64-1 CAPLUS
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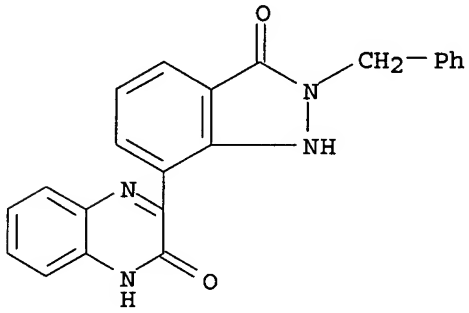
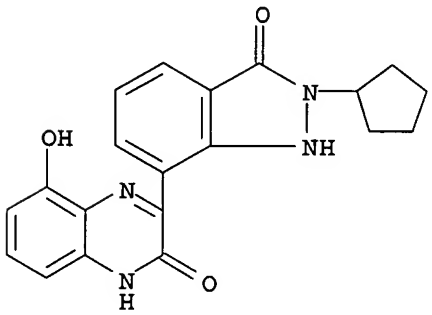
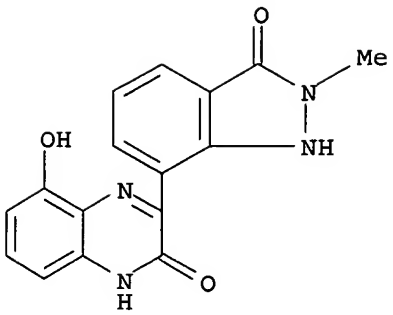


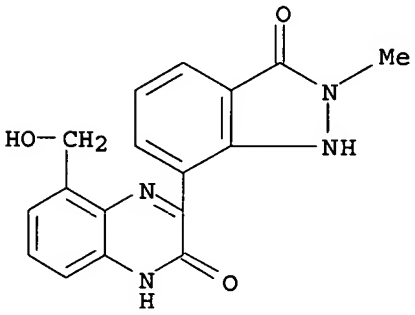
RN 388612-50-8 CAPLUS
CN 2(1H)-Quinoxalinone, 3-(2-cyclopentyl-2,3-dihydro-3-oxo-1H-indazol-7-yl)-5-hydroxy- (9CI) (CA INDEX NAME)



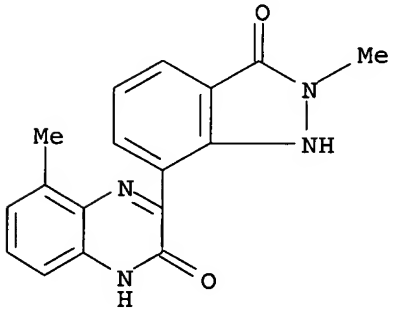
RN 388612-52-0 CAPLUS
CN 2(1H)-Quinoxalinone, 3-(2,3-dihydro-2-methyl-3-oxo-1H-indazol-7-yl)-5-hydroxy- (9CI) (CA INDEX NAME)



RN 388612-54-2 CAPLUS
CN 2(1H)-Quinoxalinone, 3-(2,3-dihydro-2-methyl-3-oxo-1H-indazol-7-yl)-5-(hydroxymethyl)- (9CI) (CA INDEX NAME)



RN 388612-56-4 CAPLUS
CN 2(1H)-Quinoxalinone, 3-(2,3-dihydro-2-methyl-3-oxo-1H-indazol-7-yl)-5-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

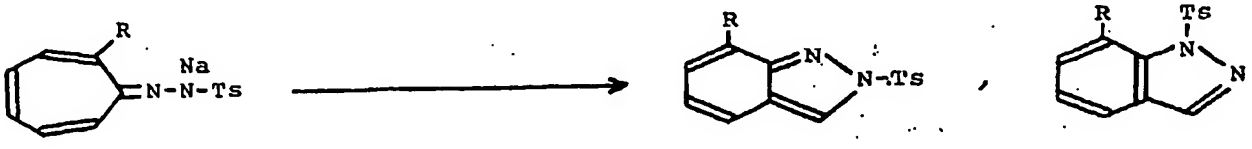
(CR)

ELECTROCHEMICAL FORMATION OF INDAZOLES FROM TROPONE TOSYLHYDRAZONES: ELECTROCHEMICAL OXIDATIONS OF SODIUM SALTS OF TOSYLHYDRAZONES OF TROPONE AND 2-PHENYLTROPONE

Katsuhiro Saito,* Masashi Hattori, Tatsuji Sato, and Kensuke Takahashi
Department of Applied Chemistry, Nagoya Institute of Technology, Gokiso-cho, Showa-ku, Nagoya 466, Japan

Abstract —— Electrochemical oxidations of the sodium salts of tropone and 2-phenyltropone tosylhydrazones afforded 2-tosyl-2H-indazole and 1-tosyl-7-phenyl-1H-indazole, respectively. The reactions proceeded through the cyclizations of the corresponding hydrazyl radicals generated by electrochemical one electron oxidations of the hydrazone anions.

Much attention has been paid to electrochemical reactions of organic compounds not only from the viewpoint of synthetic utilities but also from elucidation of the reaction mechanisms.[1] The electrochemical reactions of nitrogen atom-containing compounds such as amines, imines, and hydroxylamines have been revealed to proceed mainly through one electron oxidation of the lone pair electrons on the nitrogen atoms.[2] There is, however, a paucity on the papers dealing with the electrochemical reactions of hydrazones. And it is hard to find any document except for the electrochemical dimerization through cation radicals formed by one electron oxidation.[3]

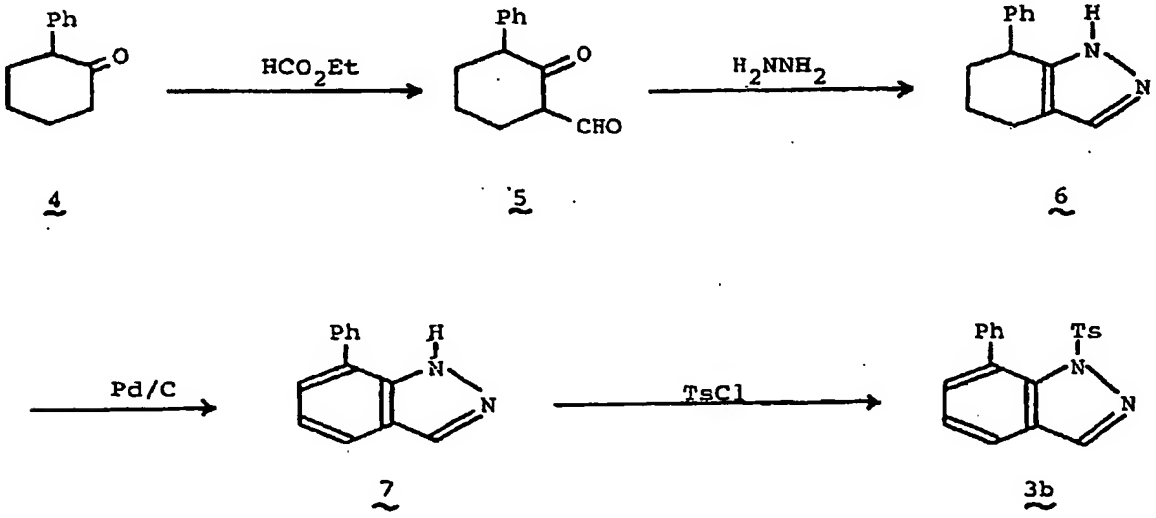


1a: R=H
b: R=Ph

2 3

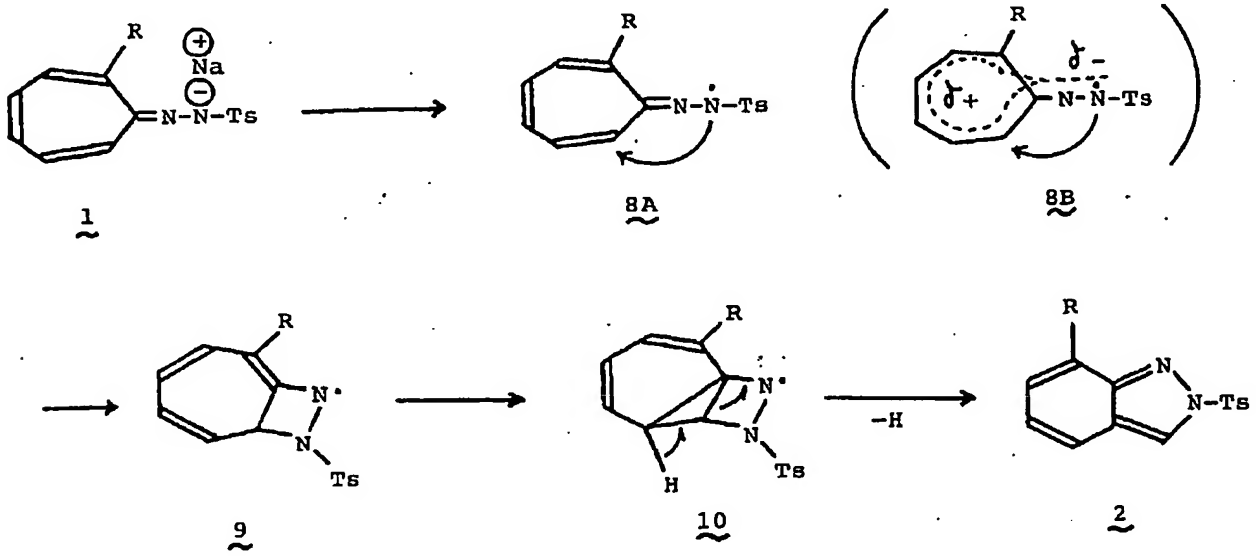
Sodium salts of tropone tosylhydrazones (1) are known to generate cyclic carbenes (cycloheptatrienylidene) or cyclic allenes (cycloheptatetraene) and their thermal and photochemical reactivities have been elucidated in very detail.[4, 5] However, we are unaware of any work concerning the electrochemical reactivities of these hydrazones. As a part of a series of our researches on the reactivities of tosylhydrazones,[5-7] we investigated into the electrochemical oxidation reactions of the sodium salts of tropone tosylhydrazones (1) affording indazole derivatives. The results are reported herein.

A solution of tropone tosylhydrazone sodium salt (1a) in anhydrous N,N-dimethylformamide (DMF) was electrolyzed in the presence of tetrabutylammonium perchlorate as a supporting electrolyte with a platinum wire as a cathode, a platinum gauze as an anode, and a silver wire as a reference electrode at + 0.6 V at room temperature under a nitrogen stream. After evaporation of the solvent under a reduced pressure, the reaction mixture was chromatographed on silica gel to give 2-tosyl-2H-indazole (2a) in 28% yield. A similar reaction on 2-phenyltropone tosylhydrazone sodium salt (1b)[8] at +1.1 V afforded 1-tosyl-7-phenyl-1H-indazole (3b) in 17% yield.[9]



The structure of 2a was determined by the coincidence of the spectral properties and melting point to those of the authentic sample.[7] The structure of 3b was also determined by the coincidence of it's melting point and spectral properties to those of the authentic sample, which was synthesized from 2-phenylcyclohexanone (4) via 2-oxo-3-phenylcyclohexanonecarbaldehyde (5), 4,5,6,7-tetrahydro-7-phenyl-1H-indazole (6), and 7-phenyl-1H-indazole (7).[10]

The formation of 2 can be speculated to proceed as follows. Electrochemical one electron oxidation of 1 forms a hydrazyl radical (8), which cyclized to give a cycloheptatriene-type intermediate (9). The ionic form (8B) is thought to contribute to this cyclization process through an interaction between the counter electric charges. A norcaradiene-type valence tautomer (10) openes its cyclopropane ring forming 2.[7,11]



ACKNOWLEDGEMENT

The authors are indebted to Professors Kaname Ito and Shoichiro Ikeda of Nagoya Institute of Technology for their fruitful suggestions.

EXPERIMENTAL

The anode was a platinum gauze of a size of 5 cm depth and 12 cm width which was separated from the cathode compartment by means of a medium-porosity sintered glass frit. The cathode was a platinum wire and the reference electrode was a silver wire. The controlled potential power was supplied from a Yanaco Potentio/Garvanostatic Electrolyser VE-9 apparatus. Melting points were recorded on a Yanagimoto Micro Melting Point Apparatus and were uncorrected. Nmr spectra were measured with Varian XL 200 spectrometer with tetramethylsilane as an internal standard. Ir and uv spectra were measured with JASCO FT/IR 5300 and Hitachi 200-10 spectrophotometers, respectively. Ms spectra were measured with a Hitachi M-2000S spectrometer.

Electrolysis of 1a. A solution of 1a (590 mg, 2 mmol), tetrabutylammonium perchlorate (6840 mg, 20 mmol) in DMF (200 ml) was electrolyzed under a nitrogen stream at room temperayure at +0.6 V. After removing the solvent by distillation under a reduced pressure (62°C, 5 mmHg) the resulting residue was chromatographed on silica gel to give colorless crystals (2a) (150 mg, 28%, mp 140°C, lit.,[7] mp 140°C, hexane-ethyl acetate (8:2)) and red crystals of tropone tosylhydrazone (110 mg, 13%, hexane-ethyl acetate (1:1)).

Electrolysis of 1b. A solution of 1b (780 mg, 2 mmol), tetrabutylammonium perchlorate (6840 mg, 20 mmol) in DMF (200 ml) was electrolyzed at +1.05 V under the same reaction conditions as above to give brown crystals (3b) (130 mg, 17%) from elution with hexane-ethyl acetate (8:2) on silica-gel chromatography.

3b: mp 94-96°C. Hrms: m/z 348.0944. Calcd for $C_{20}H_{16}N_2O_2S$: m/z 348.0943. Ms m/z (rel intensity): 348 (M^+, 100), 284 (63). Uv (MeOH): 239 nm (log ε, 4.33), 273 (3.96), 276 (3.98), 293 (3.86), 330 (3.86). Ir (KBr): 3030, 2950, 1385, 1192, 1059 cm^{-1}. ^1H Nmr ($CDCl_3$) δ 2.40 (s, 3H), 7.15-7.64 (m, 8H), 7.93-8.04 (m, 4H), 8.70 (s, 1H). ^{13}C Nmr ($CDCl_3$) δ 21.7, 120.2, 122.6, 124.3, 124.6, 127.1, 127.8, 128.4, 128.7, 128.8, 130.0, 130.1, 131.6, 133.6, 137.3, 146.3.

Synthesis of 3b. To a solution of 4 (1740 mg, 10 mmol) and ethyl formate (1110 mg, 15 mmol) in anhydrous ether (40 ml) were added sodium metal (230 mg, 10 mmol) and one drop of ethanol. After stirring at room temperature for 24 h ethanol (1 ml) was added and the mixture was further stirred for 1 h. The reaction mixture was washed with water, and dried over anhydrous sodium sulfate. Evaporation of the solvent and separation of the residue with chromatography (silica gel, ether) afforded 2-oxo-3-phenylcyclohexanonecarbaldehyde (5) as a yellow oil (1790 mg, 89%).

5: Hrms: m/z 202.0980. Calcd for $C_{13}H_{14}O_2$: m/z 202.0992. Ms m/z (rel intensity): 202 (M^+, 100), 174 (56), 146 (35). Ir (oil): 3030, 2940, 1712 cm^{-1}. ^1H Nmr ($CDCl_3$) δ 1.33-2.22 (m, 5H), 2.38-2.55 (m, 2H), 3.57-3.73 (m, 1H), 7.03-7.41 (m, 5H), 8.85 (s, 1H). ^{13}C Nmr ($CDCl_3$) δ 20.4, 23.2, 31.1, 47.2, 109.5, 126.5, 128.1, 128.2, 141.5, 182.9, 189.2.

To a solution of 5 (1410 mg, 7 mmol) in methanol (10 ml) was added hydrazine hydrate (350 mg, 7 mmol) dropwisely and the mixture was stirred at room temperature for 30 min. After evaporation of the solvent the residue was chromatographed (silica gel, hexane-ethyl acetate (3:2)) to afford colorless crystals of 4,5,6,7-tetrahydro-7-phenyl-1H-indazole (6) (1260 mg, 91%).

6: mp 115-116°C. Hrms: m/z 198.1156. Calcd for $C_{13}H_{14}N_2$: m/z 198.1156. Ms m/z (rel intensity): 198 (M^+, 100), 169 (54), 143 (18). Ir (KBr): 3159, 2928, 1493 cm^{-1}. ^1H Nmr ($CDCl_3$) δ 1.62-2.32 (m, 5H), 2.50-2.68 (m, 2H), 3.88-4.07 (m, 1H), 7.04-7.38 (m, 6H). ^{13}C Nmr ($CDCl_3$) δ 20.4, 21.9, 33.9, 40.0, 115.9, 120.4, 120.4, 127.9, 128.4, 133.4, 143.4, 144.3.

A mixture of 6 (200 mg) and palladium-carbon (5%, 85 mg) in decalin (2.5 ml) was refluxed for 24 h. The reaction mixture was chromatographed (silica gel, hexane-ethyl acetate (3:2)) to give colorless crystals (7) (140 mg, 70%).

7: mp: 151-153°C. Hrms: m/z 194.0833. Calcd for $C_{13}H_{10}N_2$: m/z 194.0843. Ms m/z (rel intensity): 194 (M^+, 100), 167 (30). Uv (MeOH): 266 nm (log ε, 3.98), 301 (4.06). Ir (KBr): 3258, 3030, 2950, 1429 cm^{-1}. ^1H Nmr ($CDCl_3$) δ 7.23-7.78 (m, 9H), 8.08 (s, 1H). ^{13}C Nmr ($CDCl_3$) δ 119.9, 121.5, 124.6, 126.0, 127.7, 127.8, 127.9, 129.2, 135.3, 138.0, 138.8.

A solution of 7 (17 mg, 0.09 mmol) and tosyl chloride (170 mg, 0.9 mmol) in pyridine (5 ml) was heated at 118°C for 2.5 h. The mixture was diluted with benzene, washed with water, and dried over anhydrous sodium sulfate. After filtration the solvent was removed on a rotary evaporator and the residue was chromatographed (silica gel, hexane-ethyl acetate (4:1)) to give brown crystals (3b) (14 mg, 46%).

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2-tosyl-2H-indazole (2a) has been reported to be formed in the reactions of opone tosylhydrazone or its sodium salt (1a) with silver chromate at 120°C.[7] wev r, the similar rections on 2-phenyltropone tosylhydrazone or its sodium lt (1b) did not afford the corresponding products, 2-tosyl-7-phenyl-2H-indazole b) or 1-tosyl-7-phenyl-1H-indazole (3b), but gave 27% yield of 2,2'-diphenyl-ptafulvalene (11), which was formed by dimerization of the carbene generated by ermolysis of 1b.

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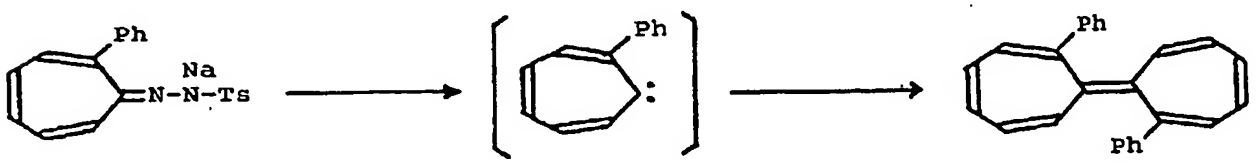

1b 11

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Received, 17th October, 1991

L12 ANSWER 31 OF 43 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:214408 CAPLUS
DOCUMENT NUMBER: 116:214408
TITLE: Electrochemical formation of indazoles from tropone tosylhydrazones: electrochemical oxidations of sodium salts of tosylhydrazones of tropone and 2-phenyltropone
AUTHOR(S): Saito, Katsuhiro; Hattori, Masashi; Sato, Tatsuji; Takahashi, Kensuke
CORPORATE SOURCE: Dep. Appl. Chem., Nagoya Inst. Technol., Nagoya, 466, Japan
SOURCE: Heterocycles (1992), 34(1), 129-34
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:214408
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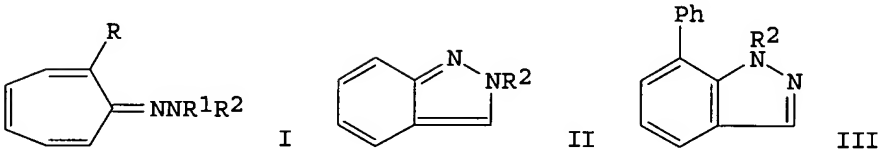
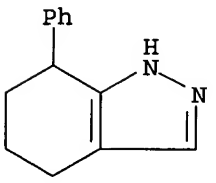
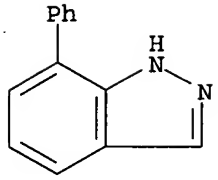


AB Electrochem. oxidation of the sodium salts I (R = H, Ph, R1 = Na, R2 = tosyl) of tropone and 2-phenyltropone tosylhydrazones afforded 2-tosyl-2H-indazole II and 1-tosyl-7-phenyl-1H-indazole III (R2 = tosyl), resp. The reactions proceeded through the cyclization of the corresponding hydrazyl radicals generated by electrochem. one-electron oxidation of the hydrazone anions.

IT **141037-87-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and catalytic dehydrogenation of)
RN 141037-87-8 CAPLUS
CN 1H-Indazole, 4,5,6,7-tetrahydro-7-phenyl- (9CI) (CA INDEX NAME)



IT **141037-88-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and N-tosylation of)
RN 141037-88-9 CAPLUS
CN 1H-Indazole, 7-phenyl- (9CI) (CA INDEX NAME)



IT **141037-86-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 141037-86-7 CAPLUS
CN 1H-Indazole, 1-[(4-methylphenyl)sulfonyl]-7-phenyl- (9CI) (CA INDEX NAME)